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Maintenance and Testing of Hydrological Simulation Program--FORTRAN (HSPF)

Hydrocomp, Inc.
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MAINTENANCE AND TESTING OF HYDROLOGICAL SIMULATION PROGRAM--FORTRAN (HSPF)

by

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The Hydrological Simulation Program--FORTRAN is a mathematical model that simulates hydrology and water quality in natural and man-made water systems. This report describes the work involved in maintaining and testing HSPF over a one-year period following its initial development An account is given of the chronology of major events during the maintenance work. The testing included work with hypothetical data and checks against outputs produced by three predecessor models, the ARM, NPS, and HSP-QUALITY models. Through this process it was determined that the HSPF model functioned as designed.

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FOREWORD

As environmental controls become more costly to implement and the penalties of judgment errors become more severe, environmental quality management requires more efficient analytical tools based on greater knowledge of the environmental phenomena to be managed. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Technology Development and Applications Branch develops management and engineering tools to help pollution control officials achieve water quality goals through watershed management.

The development and application of mathematical models to simulate the movement of pollutants through a watershed and thus to anticipate environmental problems has been the subject of intensive EPA research for several years. The most recent advance in this modeling approach is the Hydrological Simulation Program--FORTRAN (HSPF), which uses digital computers to simulate hydrology and water quality in natural and man-made water systems. HSPF is designed for easy application to most watersheds using existing meteorologic and hydrologic data. Although data requirements are extensive and running costs are signinicant, HSPF is thought to be the most accurate and appropriate management tool presently available for the continuous simulation of hydrology and water quality in watersheds.

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ABSTRACT

The Hydrological Simulation Program--FORTRAN (HSPF) is a mathematical model that simulates hydrology and water quality in natural and man-made water systems. This report describes the work involved in maintaining and testing HSPF over a period of one year following its initial development. An account is given of the chronology of major events during the maintenance work. One of the major lessons learned was that the preparation of a new release of the code and documentation is more costly than first expected. The testing included work with hypothetical data and checks against outputs produced by three predecessor models, the ARM, NPS, and HSP-QUALITY models. Through this process, it was determined that the HSPF model functioned as designed.

This report was submitted in partial fulfillment of Contract No. 68-01-5801 by Hydrocomp, Inc., under the sponsorship of the U.S. Environmental Protection Agency. This report covers the period March 1979 to June 1980, and work was completed as of June 1980.

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1.0 INTRODUCTION

The purpose of the work described in this report was to maintain and test the Hydrological Simulation Program-FORTRAN (HSPF), which had previously been developed under EPA sponsorship.

HSPF is a mathematical model for simulating the hydrologic and water quality processed in and under the land surfaces of a watershed and in the associated streams and lakes. The roots of HSPF go back to the famous Stanford Watershed Model (Crawford and Linsley 1966), which was one of the first rainfall-runoff computer models and was developed under National Science Foundation sponsorship. Many newer models have been developed from it; among the best known is the Hydrocomp Simulation Program (Hydrocomp Inc. 1969), which incorporated a sophisticated time series management system. Hydrocomp also developed a water quality model (Hydrocomp Inc. 1977) which simulates the accumulation of constituents on a watershed surface, their washoff into streams and lakes and the biochemical transformations that occur in such water bodies.

The "Lands" section of the Stanford Watershed Model was also used as the basis for the Agricultural Runoff Management (ARM) Model (Crawford and Donigian 1973, Donigian and Crawford 1976 a, and Donigian et al 1977) which was sponsored by the U.S. EPA through the Environmental Research Laboratory in Athens, Georgia. It simulates sediment production, as well as the behavior of pesticides and nutrients, on agricultural lands. The U.S. EPA also sponsored the development of the Non-Point Source (NPS) Model (Donigian and Crawford 1976 b) which simulates the washoff of constituents from land surfaces by relations with washed off sediment.

Although all the above models originated from the Stanford Watershed Model, they have each undergone develpment in their own specialized directions. Each one is a powerful tool for use in its area of specialization, but it is

not easy to use them together in situations where their combined strength is required. With the goal of overcoming this problem, the Environmental Research Laboratory (ERL) in Athens, Georgia sponsored the development of a "comprehensive package for the simulation of watershed hydrology and water quality", which later became known as HSPF. The objective was to incorporate the capabilities of all of the above models in a single, consistently designed set of well-documented software, written as far as possible in ANSI FORTRAN (1966 Version). This was part of the ERL's program to develop engineering tools to help pollution control officials achieve water quality goals through watershed management.

Work on the development of HSPF, under Grant No. R804971-01, started in November 1976 and ended in Novenber 1978. In February 1979 the go-ahead was received to commence work on the present maintenance and testing contract. This work culminated with the issue of Release 5 of the code (in February 1980), a revised User's Manual (Johanson, et. al. 1979) and this report.

2.0 CONCLUSIONS

Our conclusions relating to the maintenance phase of this project are:

1. The care which went into the design, coding, and documentation of the HSPF software is paying off; it is relatively easy for a well-trained person to maintain. Bugs have usually been easy to locate and to fix. It has also been easy to add new modules, as envisaged in the design.

2. Implementation on a wide variety of machines is more difficult than originally envisaged. This is due principally to two factors:

   a. The sheer size of the system, which makes it impossible to implement on certain machines and/or operating systems (e.g., PDP11 with IAS).

   b. The use of half-word integers. This extension to ANSI FORTRAN is not implemented on some widely used machines. In retrospect, we believe this extension should not have been used.

3. We have been able to maintain high standards in:

   a. Keeping the code consistent with the principle of Structured Programming Technology.

   b. Keeping the documentation and other associated datasets consistent with the code.

This consistency was quite costly, since the logistics of maintaining a large system, with 500 subroutines and a user's manual of 650 pages, are quite complex. It required continuous effort and great attention to detail.

4. In the future, as the number of users increases, most of the maintenance work will consist of:

   a. Answering questions while users are still installing or becoming accustomed to HSPF. Many users are likely to have initial difficulties, particularly if they have not attended a workshop. Most of these calls will not involve bugs in the code.

   b. Updating of code, documentation, and associated datasets, (i.e., New Releases), if significant alterations or enhancements are made to the system.

   c. Communication of information to users, through a monthly or quarterly circular.

5. Because of the great flexibility of HSPF and the fact that it makes extensive use of disc input/output, it takes more computer time (and dollars) than did its predecessor models.

6. It was wise to restrain wholesale distribution of the system until the testing work was complete.

Our conclusions relating to the testing phase of this work are:

1. HSPF has been put through a comprehensive set of tests and found to correctly implement the algorithms described in the User's Manual. It is ready for public distribution.

2. Where it was checked against its predecessor models, HSPF produced similar output, with these notable exceptions:

   a. Simulation of nutrient behavior in pervious land segments (PERLND module) did not agree with the results produced by the ARM model. This is attributable to:

      (i) Intermittent calculation of reaction fluxes in ARM Model runs

      (ii) Problems inherent in having a thin surface layer, with moisture storage dependent only on overland flow depth (a feature of both ARM and HSPF)

   b. Simulation of phytoplankton in streams and reservoirs. Because HSPF and HSP-QUALITY use different definitions of "water body depth" in the light extinction equation, they produce radically different light-limiting phytoplankton growth rates.

3.0 RECOMMENDATIONS

1. The EPA should publicize the HSPF system, stressing its great flexibility in operation and its many other unique features, many of which are not obvious to a casual user. This publicity could include partial or full sponsorship of additional workshops, for new or experienced users.

2. The EPA should continue to support the program through:

   a. Help for new users who are experiencing difficulty in installing or understanding the system.

   b. Maintenance of "official" and "development" versions of the code, documentation, and associated datasets.

   c. Correction of bugs reported by users, periodic reporting of such information and production of new releases when necessary.

3. The EPA should consider sponsoring some further development of the model:

   a. Elimination of half-word integers, to make it easier to install on a variety of machines.

   b. Development of a special version for large-memory installations, designed to minimize disc input/output and associated costs.

   c. Improved trapping of user's errors, by the Run Interpreter.

   d. A study of the feasibility of having a dynamically varying internal time step for certain processes - fine when there is rapid

variation, coarse when there is not. This would save computer time.

4. Two problems in the agricultural chemical simulation system of the PERLND module need to be solved:

   a. The MSTLAY section needs to be reformulated, so that the system will give results that are not a direct function of the time step, thus freeing this part of HSPF from the 5 and 15 minute time steps to which it (and ARM) is limited.

   b. The problems posed by the use of a thin surface layer, with moisture storage totally dependent on overland flow depth, must be overcome.

5. A short series of tests designed to check the following should be considered:

   a. The effect of varying the internal time step.

   b. The effect of varying the number of "areal-source blocks" in the PERLND module.

4.0 MAINTENANCE EXPERIENCE

4.1 SCOPE OF MAINTENANCE WORK

The EPA set out its requirements for this task in its "request for proposal" (RFP), issued in January 1979. In our proposal (February 1979) we responded to these points and expanded on them. Later, there was some further negotiation on the items to be included in the maintenance and the testing tasks. The maintenance work was finally divided into four principal categories:

1. New Installations. For services to be provided, at EPA's request, in setting up the HSPF system on other computer installations.

2. Bug Correction. For work involved in correcting errors found in the code.

3. New Releases. For work involved in producing new versions of the code (incorporating the latest updates) and associated revisions to the documentation.

4. Software Extension. For work involving the addition of new capabilities to the package.

4.2 NEW INSTALLATIONS

When this contract commenced it was envisioned that HSPF would be distributed quite widely while the testing work was still in progress and that Hydrocomp would provide some assistance in installing HSPF at other computer centers, as part of this contract. It was stipulated that the service was to be provided only to public agencies or their consultants, at

the request of EPA, and that the total time spent was not to exceed two weeks.

As work progressed, the dangers involved in distributing a relatively untested set of code became apparent and EPA wisely decided to limit distribution until the testing work was complete. As a result, Hydrocomp has provided assistance to only two organizations as part of this contract:

1. ERL-Athens. When this project commenced, we sent a copy of the FORTRAN code to ERL Athens, for possible installation on their PDP11 system. As expected, the FORTRAN language used on our HP3000 machine was easy to adapt to the PDP11 installation, but the program was too large to be handled by the operating system available there. And, since it was not practical to install an alternative operating system, EPA needed a version of the code which could run on the IBM370 system provided by its computing vendor in Washington, D.C. This need coincided with a similar request from a different client. Thus, an IBM version of the code (called Release 3) was produced during May and June 1979, and sent to ERL-Athens in July, where it was installed with little difficulty.

2. By November, 1979 Release 4 of the code was available. At EPA's request, we supplied a copy to their contractors for the Iowa field evaluation program. They installed it without difficulty at Stanford University and forwarded a copy to ERL-Athens.

In February 1980 the final release of the code and documentation was available. A copy was sent to the Project Officer for installation at EPA, and for general distribution.

During the past year we have also distributed copies of the code to some other clients, by private arrangements. Some private arrangements for maintenance and applications assistance have also been made. This work has

benefited the present contract because experience gained in these situations has made possible some improvements to the whole HSPF package.

Although only two "new installations" were serviced under this contract during the past year, the need for this kind of assistance will almost certainly increase in the future, and we believe EPA should continue to provide some such service. Based on our experience thus far, with public and private distribution, most users do not require extensive help if they are installing HSPF on a type of system on which it has already been checked out (HP3000, IBM360 or 370). A few phone calls are usually all that is necessary.

In this connection, EPA should consider sponsoring some work to make HSPF available on a wider range of machines:

1. Elimination of the use of half-word integers. In retrospect, we can see that their use has not been beneficial; adaptation of HSPF to systems like UNIVAC 1100, CDC, and Honeywell would be greatly assisted if half-word integers were eliminated.

2. Development of a version tailored for larger machines. At present, the COMMON block is of limited size, to permit the system to operate on smaller machines. By enlarging the COMMON block, the frequency of disc input/output could be considerably reduced. This would greatly assist users who presently find HSPF too expensive to run because of disc I/O charges.

4.3 BUG CORRECTION

This subtask covered the work involved in fixing errors reported by users. Typically, when a user experienced a problem, we would first have to check whether the problem was due to a bug or to an error in the way he had set up his input. If a bug was found, the FORTRAN code was suitably altered, the affected subprogram(s) recompiled and the entire system relinked. Any associated alterations to the pseudo code and User's Manual were noted, but their implementation was deferred until a sufficient number of changes had been accumulated to warrant the issue of a new release of the system (covered under "New Releases" subtask).

Because initial distribution of the program was limited, the vast majority of bugs were reported by Hydrocomp employees who were working on the testing phase of this project and a variety of other projects which made use of HSPF. However, some bugs were first discovered by other users.

The rate at which bugs were found decreased with time, as expected. Initially, we projected that there would not be a corresponding decline in the rate of expenditure on this subtask because the bugs would become progressively more subtle and difficult to fix. However, this was not the case. In general, the later bugs have been no more difficult to locate and fix than were the earlier ones. Thus, the effort expended on this subtask did decrease progressively, from eleven person-days in April '79 to six in June, and 1.5 in November. It should be noted that this experience applies primarily to bugs reported within our own organization. It is not applicable to problems encountered by other users because:

1. It can be quite difficult to obtain sufficient information from the user to judge whether the problem is of his own making or is, indeed, due to a bug in the program.

2. The bug might be specific to a certain version of the program. For example, we had at least one problem reported to us which occurred only on the IBM version of the code. It took some time and effort to diagnose and correct the problem, since we:

   a) had to obtain copies of the user's input (on tape)

   b) first tried running it on our installation, and found no problem

   c) switched to an IBM installation, and diagnosed the problem there

We mention the above points because they are especially relevant to future maintenance sponsored by EPA. It will often be difficult to determine whether a user's problem is due to an error in the code and, if so, to locate it, fix it, and notify all other affected users of the problem.

In retrospect, we can see that it was wise to limit the circulation of the model until the completion of testing. If EPA had not done so, much effort would have been expended in dealing with problems encountered by users working with partially tested code. As it happened, most of the problems were found by users in our own organization, and could be quickly dealt with because communication was quick and complete.

The RFP for this contract (and our proposal) envisaged the production of a monthly circular to inform users of bugs (and work-arounds for them, where possible). Because of the limited circulation of HSPF during this project, the circular was not necessary. However, in the future a monthly (or

perhaps quarterly) circular would serve a useful purpose.

4.4 NEW RELEASES

General Approach

Our approach to this work is similar to that adopted by most computer companies who support software. It starts with the premise that the computer code will evolve, as bugs are fixed, new options added, etc. It is also presumed that the documentation should be kept consistent with the code.

Obviously, it is not economical to issue a new copy of the code and documentation every time a change is made. Rather, one should accumulate (and test) the changes until enough have been collected to justify the issue of a new "release" of the code. To do this effectively, the maintainer must keep at least two versions of the code on his computer system:

1. The latest official release. This would be the version normally sent to any user who requests a copy of the software.

2. A "development version". This version includes all updates and extensions made since the last release, and is normally only used within the maintainer's organization, to collect and test the updates.

A parallel system is used to keep the documentation in step with the code. Between issues of official releases, users should be notified of any significant problems in the latest official version via a newsletter or circular.

Mechanism Used to Generate a New Release

Whenever we decided to issue a new release, the following steps were involved:

1. All files containing FORTRAN code, load modules, etc., in the "development" state were now designated the new "official" version and given a new release number. The old version was purged.

2. Many associated datasets, containing the documentation, pseudo code, data structures, sample JCL, etc. had to be updated. While the new version was under development, the updates to these files had simply been marked on listings - now all the updates were actually performed.

3. New and/or updated pages for the User's Manual were prepared, as well as an "Errata Sheet" containing minor changes that did not warrant reissue of an entire page.

4. All new and revised datasets were copied to tape, to provide a backup.

5. An "IBM version master tape" was created, by running a program that automatically generated IBM FORTRAN from HP3000 FORTRAN.

History of Activities

As soon as work on this contract started in February 1979, there was intense activity on the testing and development of the HSPF system. As a result, the System Documentation which had been produced in December 1978 soon lagged far behind the state of the FORTRAN code and became out of date. Then, from May through August, attention was shifted away from the testing and debugging work, so that the documentation could be completely revised. (This work proceeded simultaneously with the development of the IBM version

of the code.) With the concurrence of the Project Officer, it was decided to divide the documentation into two publications:

1. The User's Manual (650 pages). This would contain all the information that a user would normally require and would be printed and distributed by EPA.

2. The Programmer's Supplement. This would contain additional documentation, such as the pseudo code and data structures, which would be useful to those who need to understand the inner workings of HSPF or who need to modify or extend it. For the sake of economy, it was decided not to print this information but to circulate it on magnetic tape with the source code and other associated datasets.

This extensive overhaul of the documentation and the development of the IBM version culminated in the issue of Release 3 of the code and documentation, dated September 1979. The originals for the User's Manual were sent to EPA so that arrangements for printing could be put in hand while the development and testing continued.

The next release was issued in November 1979. It included the new utility modules (DISPLY, DURANL, AND GENER), which had been developed during September and October as part of the "Software Extension" subtask. It was issued to provide the EPA, its contractors, and Hydrocomp clients with an updated interim version of the code, seeing that the final release was only due for issue in February 1980.

Release 5 was issued in February. Tapes containing the source code, Programmer's Supplement, and all associated datasets were sent to the Project Offier. These were the principal deliverable items in this contract. Updates for the User's Manual were also sent.

Summary and Conclusions

In retrospect, it seems we were right to issue three new releases during the course of the project. The model was undergoing relatively rapid change through this development and testing period, so each release did contain a very significant quantity of different material to the previous one. From now on, the frequency should be far lower because we know the code and documentation are thoroughly checked out and very reliable. We suggest that EPA might issue a new release once or twice per year and handle changes in the interim by circulating notices to users wherever necessary. However, if significant alterations or additions to the program are planned, the frequency of new releases would need to be higher.

The main surprise in doing this work was the high cost of preparing and maintaining good quality documentation. In our proposal, "New Releases" was scheduled to take about 12% of the total maintenance effort. The actual cost was about 50%. The ratio is likely to remain at about this level in the future because of the logistical problems involved when there are many users, on different computer systems, to be serviced (we include the cost of preparing the periodic newsletter in this estimate).

The high cost of keeping good, consistent master copies of code and documentation probably accounts for the fact that engineering programs are often not well documented and that no official copy is kept--users are left to fend for themselves. This is, indeed, an alternative philosophy of software "maintenance" and distribution. But we believe that EPA should plan to support an official copy.

4.5 SOFTWARE EXTENSION

HSPF was designed so that new or alternative operating modules could be added to the system with relatively little difficulty, provided the person doing the work has a thorough grasp of the basic design. There are several advantages to this aspect of the design:

1. New operating modules can send output to, or get input from, any of the existing operating modules in HSPF--the user does not have to write any "interfacing" software to achieve this.

2. The new modules can communicate with an HSPF Time Series Store, via the existing Time Series Management System (TSGET and TSPUT modules), and thus instantly gain the advantages provided by it, such as:

   a. automatic conversion of time step between the operating modules and the TSS, where necessary.

   b. the ability to read time series placed into the Time Series Store (TSS) by another module, and vice versa.

   c. the use of compressed storage of data in the TSS.

Some of the innovative design features of HSPF were expensive to provide but we expected that the flexibility that they brought would soon justify the investment. Thus, in our proposal for this contract, we suggested that for a modest additional investment some utility modules could be added, which would greatly enhance the power of the entire system.

The utility modules added to HSPF were:

1. PLTGEN. This module accepts one or more time series as inputs and generates a "plot file", in which the data are recorded sequentially. This file is then read by a stand-alone program which translates the information into commands which drive a plotter. Thus, any time series of recorded or computed data can be plotted individually or in concert with several others.

2. DISPLY. This module permits any time series to be displayed in a neatly formatted table, at any of the HSPF-supported time steps. Day, month, and annual totals, averages, etc. can also be included in the tabular layouts.

3. DURANL. This module performs a variety of statistical analyses on a time series. The simplest option produces a cumulative frequency distribution of the time series. But it can also determine the frequency of excursions (of specified durations) above or below preset levels. This option can be used to answer a question such as "How often does the concentration of constituent X exceed Y mg/l for Z or more consecutive time steps?

4. GENER. This module is used to generate a time series from one or two others. For example, it can produce a series C whose values are the natural log of those in the input time series A. Or, it can produce a time series C whose values are the product of those in two input time series A and B. This latter option could be used to compute the flow of a constituent (in load units) given the two time series of flow of water and constituent concentration. Altogether the GENER module provides for 14 different transformations.

The total cost of the software extension work was $17,000; only about $4,000 per module. We believe that this low cost does validate our contention that the design of the system makes it easy to integrate new operating modules

into HSPF. One "outside" user has added yet another utility module; also with very little effort.

5.0 TESTING

5.1 PURPOSE AND SCOPE OF TESTING

The purpose of this testing work was to check that the HSPF code correctly implemented the modeling algorithms outlined in the User's Manual. The algorithms are, for the most part, similar to those embodied in the predecessor models, but the manner in which they are included in HSPF is very different, since it has a radically different structure compared with its forebears. Thus, most of the testing consisted in comparing the output produced by HSPF against that produced by the ARM, NPS, and HSP-QUALITY models, given identical inputs. We reasoned that, if the outputs were close, the old and new models agreed with each other and, most likely, they both correctly implemented the modeling algorithms. But, if they differed substantially, there was a possibility that HSPF was in error, and the difference must be investigated.

This was a different approach to that usually taken in testing work where model output is compared against observed data. We reasoned that the predecessor models had already been checked in this way (e.g., Donigian and Crawford 1976 b, Donigian et. al. 1977). Thus, in the first instance, HSPF should be tested by checking its consistency with these models. Later, any features of HSPF which are not present in the predecessor models, or which have been intentionally implemented differently, could be tested in the usual way.

The testing work was in three phases:

1. Tests using hypothetical data. In this work the modules were set up to operate in hypothetical situations. This usually involved the use of simple input time series and parameter sets. The simulation output was checked against manual calculations.

2. Tests on data from the Occoquan basin, Virginia. In 1977, Hydrocomp developed the Occoquan Basin Computer Model (Hydrocomp 1978) for the Northern Virginia Planning District Commission (NVPDC). It incorporates the Nonpoint Source (NPS) model and the HSP-QUALITY model, plus some extensions. Since the algorithms in HSPF and the Occoquan Basin Computer Model are, for the most part, similar and, since NVPDC had performed extensive simulation work on the Occoquan Basin, their data set was an obvious choice for testing HSPF.

3. Tests on data from Michigan State University watershed P6. In 1977, we completed a project for EPA which involved the refinement and testing of the ARM model (Donigian et. al. 1977). Part of this work used data which Michigan State University (MSU) had collected on their P6 test watershed, and involved the testing of the snowmelt and agricultural chemical sections of the ARM model. This dataset was also included in the HSPF testing because the simulations performed on the Occoquan by NVPDC did not include snowmelt and the detailed simulation of pesticides and nutrients. Thus the MSU dataset filled a large gap which would otherwise have been present in our testing work.

5.2 TESTS USING HYPOTHETICAL DATA

When this contract commenced on February 20, 1979, the HSPF system was practically complete, but bugs prevented some areas of the code from operating or caused them to give incorrect results. The first task was to bring the entire package to the point where it could operate successfully and to ensure, as far as possible, that the results produced were

reasonable. To do this, a succession of at least 13 different test inputs was created, each designed to exercise a different area of the code. Using these, we steadily worked our way through the PERLND, IMPLND, and RCHRES modules. We would attempt to run a test dataset, fix any bugs which prevented execution and, once it successfully executed, check that the results were reasonable. Then we would move on to the next test. This process took place during March and April 1979. By April 15 all the HSPF code was executable.

A variety of checks were performed on the results obtained from these tests:

1. Many module sections provide an internal check, by computing a "continuity error" for each printout interval. We would examine these errors and check that they were less than 1 part in 10,000.

2. Where possible, we would check model output against a hand calculation. For example, the first RCHRES test run involved a stagnant water body 2.5 ft. deep and 1 acre in extent. We checked the behavior of the HYDR section of the module by ensuring that it gave the intended zero outflow and that all state variables (e.g., depth, durface area) remained constant, including the requirement that they not oscillate. The water temperature calculation was checked by supplying constant meteorologic data and checking that the temperature built up smoothly from the initial value to an equilibrium value. The equilibrium temperature was checked by manually evaluating all heat exchange components (long wave, short wave, etc.) at that temperature and ensuring that the resultant heat flux was zero.

The simulation of certain reactions was checked by first setting the reaction rate to zero and ensuring that the constituent was conserved. Then, we would assign a non-zero value and check that the transformation

rate was close to that predicted by hand calculation.

These tests were very useful. They were easy to set up and permitted many aspects of the model to be checked very quickly. Several of these early test setups are now used, in slightly modified form, to demonstrate HSPF in our workshop sessions.

5.3 TESTS ON DATA FROM THE OCCOQUAN BASIN

Introduction

The Northern Virginia Planning District Commission (NVPDC) kindly cooperated in this work by supplying us with all needed data, including their simulation inputs and outputs recorded on magnetic tape. The Occoquan basin (Figure 1) has been subdivided for modeling purposes into 15 "subbasins" and a similar number of stream and reservoir "reaches". Early in the testing work we realized that, conceptually, all the subbasins and reaches were identical. That is, they all involved simulation of the same sets of constituents using the same methods. Thus, when simulating them, the same set of code is executed for each one; only the numerical values are different. The implication for the testing work is that any differences between the HSPF and Occoquan Basin Computer Model (OBCM) code would probably be equally apparent in their outputs for all subbasins or reaches. There was, thus, not much to be gained by including the whole set of subbasins and reaches in the tests. The output for each subbasin or reach could be expected to tell much the same story. Therefore, with the concurrence of the Project Officer, we decided to focus attention on Broad Run (subbasins 4, 5, and 7). If we had included a greater area, the cost of manipulating the data would have risen proportionately, but there would not have been a significant increase in the payoff.

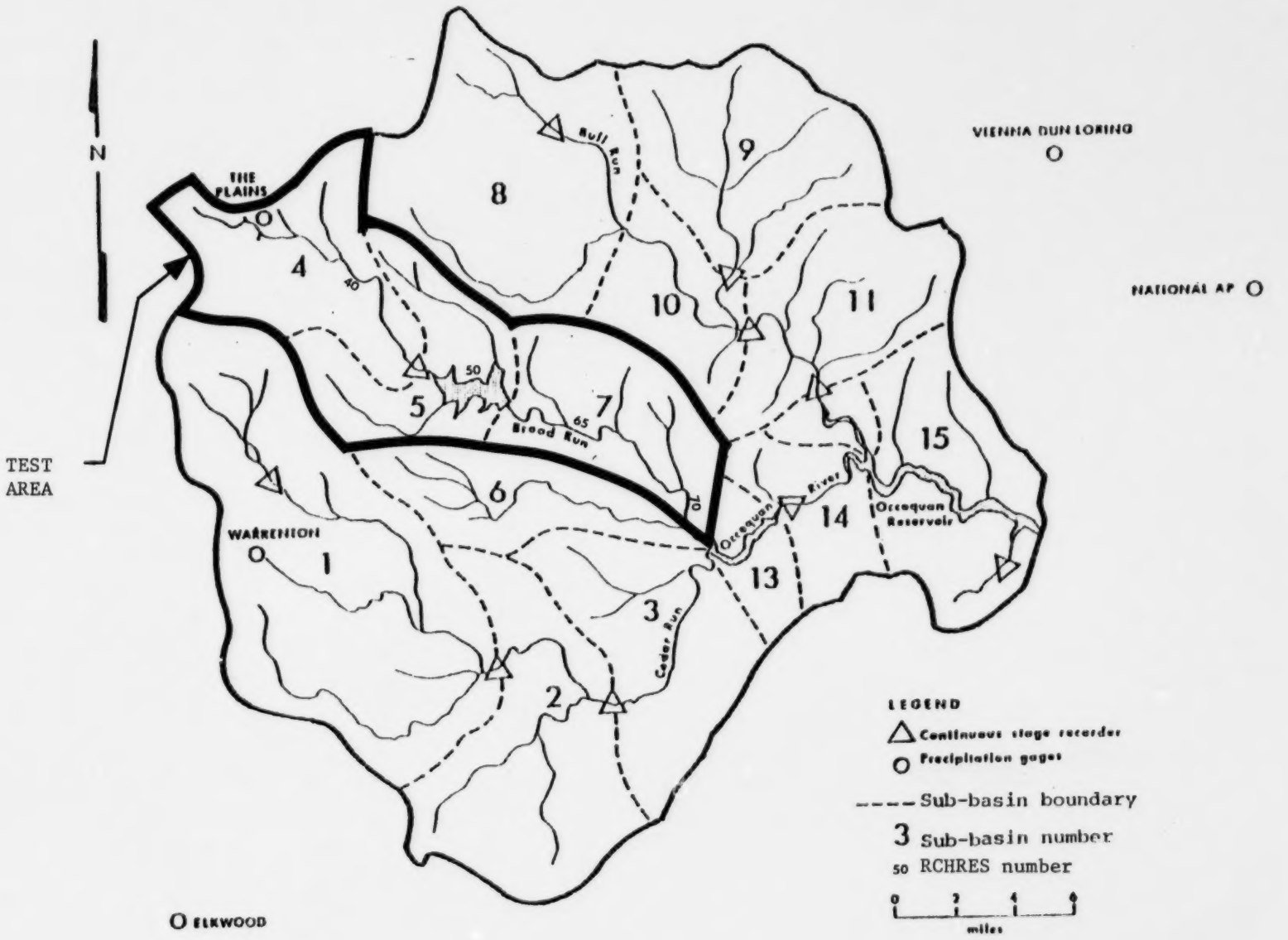


Figure 1 Map Showing Sub-basins Included in Occoquan Basin

Method

The testing sequence followed the logical pattern present in HSPF and predecessor models:

1. Simulate the land segments. Compare the runoff and constituent washoff calculated by NPS and HSPF. When the sources of any obvious differences have been tracked down, modify the HSPF code and/or the input and rerun. Repeat until the agreement is good. Store outputs from the land-segments on disc, for input to the RCHRES system.

2. Repeat the process for the stream and reservoir system.

Simulation of Land Segments

The NVPDC had divided each sub-basin into five land use classes:

> Forest/Idle Agriculture, cropping Agriculture, pasture Urban, residential Urban, "employment"

Each land use was further subdivided into a pervious and impervious fraction, as permitted by the NPS model. This subdivision presented us with a problem in constructing an HSPF input which was strictly equivalent to that for NPS. In HSPF, a land segment is regarded as an area which is really homogeneous not only with respect to hydrological behavior, but also with respect to land use, constituent potency factors, etc. In designing the model it was reasoned that different land use will, in general, be associated with different hydrological behavior and, thus, should be represented by different land segments. Thus, in HSPF, each subbasin in the Occoquan had to be represented by not one, but five, pervious land segments. Furthermore, HSPF treats impervious areas as logically distinct from pervious areas, and simulates them with a separate module (IMPLND). Thus,

the impervious fraction of each land use area identified in NPS had to be simulated in HSPF with its own impervious land segment.

The overall result was that a subbasin which could be simulated with one land segment in the NPS model had to be represented by ten land segments in HSPF, to obtain an exactly equivalent input. Inevitably, this made the HSPF User's Control Input rather cumbersome and resulted in much lower execution efficiency than would have been obtained had we segmented the subbasins in a manner more appropriate to HSPF.

The testing proceeded as follows:

1. The runoff of water, and the washoff of each constituent, as computed by NPS for each subbasin, had been written to disc.

2. The corresponding values for the HSPF simulation were found by combining the washoff from each of the ten land segments, in proportion to the area of each, and writing the result to disc.

3. The outputs were compared by plotting them together (using the PLTGEN module) and making a visual comparison. A quantitative comparison could also be made by comparing the printed outputs.

4. By examining the nature of discrepancies between the two outputs, we could usually identify the cause. Most often it was a problem in the HSPF input stream. For example, we initially used the same sediment accumulation rates in HSPF as had been used in NPS. After noticing that the HSPF model accumulated sediment more rapidly than did NPS, we realized that NPS only performs accumulation on a "non-rain day", whereas HSPF does it every day. One must therefore adjust downward the accumulation rate supplied to HSPF to get an input exactly equivalent to that for NPS. But not all differences in model output were attributable

to this kind of problem. Some did uncover bugs in the HSPF code and, in one instance, in the NPS code.

The process of tracking down problems was laborious but, in the end, excellent agreement between the two sets of output was obtained. Figures 2 through 4 show typical results.

Figure 2 shows that the hydrologic outputs of HSPF and NPS are practically identical. Figures 3 and 4 show the simulated concentration of PO4 and oranic N in the outflow from subbasin 4. For both constituents, the model inputs specified a constant "background" value for the concentration of the substance in groundwater and interflow outflow. Thus, the curves of concentration versus time can only depart from the background value when surface runoff is occurring; a relatively rare occurrence. The resulting spikes can be above or below the background value, depending on whether the simulated concentration in the surface runoff is greater than or less than the background value (in general, this is a function of the intensity of surface runoff).

The agreement between the results from the two models (Figures 3 and 4) is good. The only obvious discrepancy is a small difference in the background concentrations. This is due to data roundoff. The values simulated by the NPS model were stored in an HSP OSFILE on an IBM system. A copy was sent to us. We translated the data so that they could be read into an HSPF Time Series Store on our HP3000 computer. Some data roundoff occurred in the process of making the transfer.

Simulation of the Stream Channel/Reservoir System

The setup used to represent the Broad Run stream channels and reservoir in HSPF was similar to that used by NVPDC (Figure 1). That is, the principal channels in subbasin 4 were represented by a single free flowing reach (40),

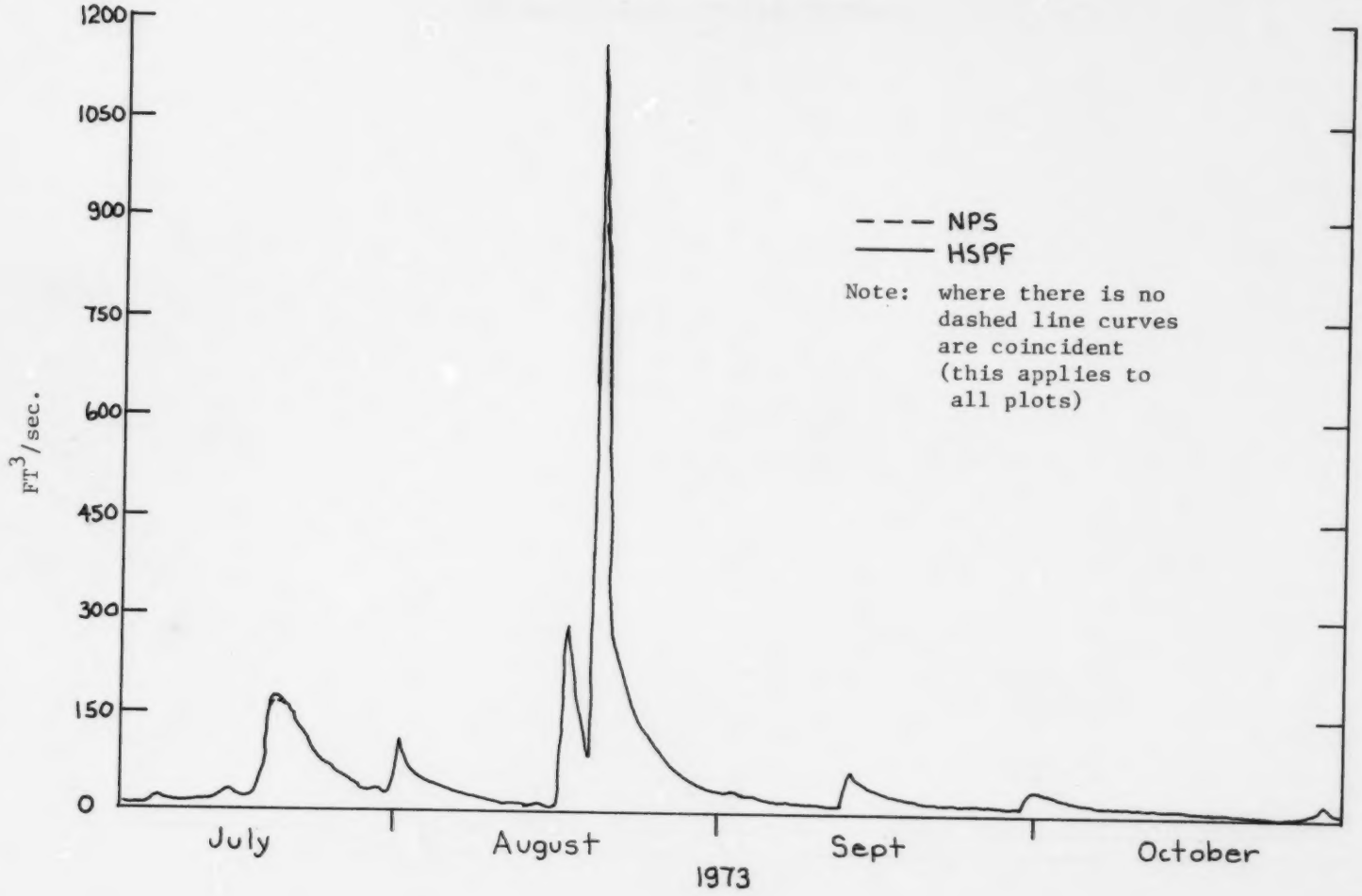


FIGURE 2 SIMULATED OUTFLOW FROM SUBBASIN 4 (OCCOQUAN)

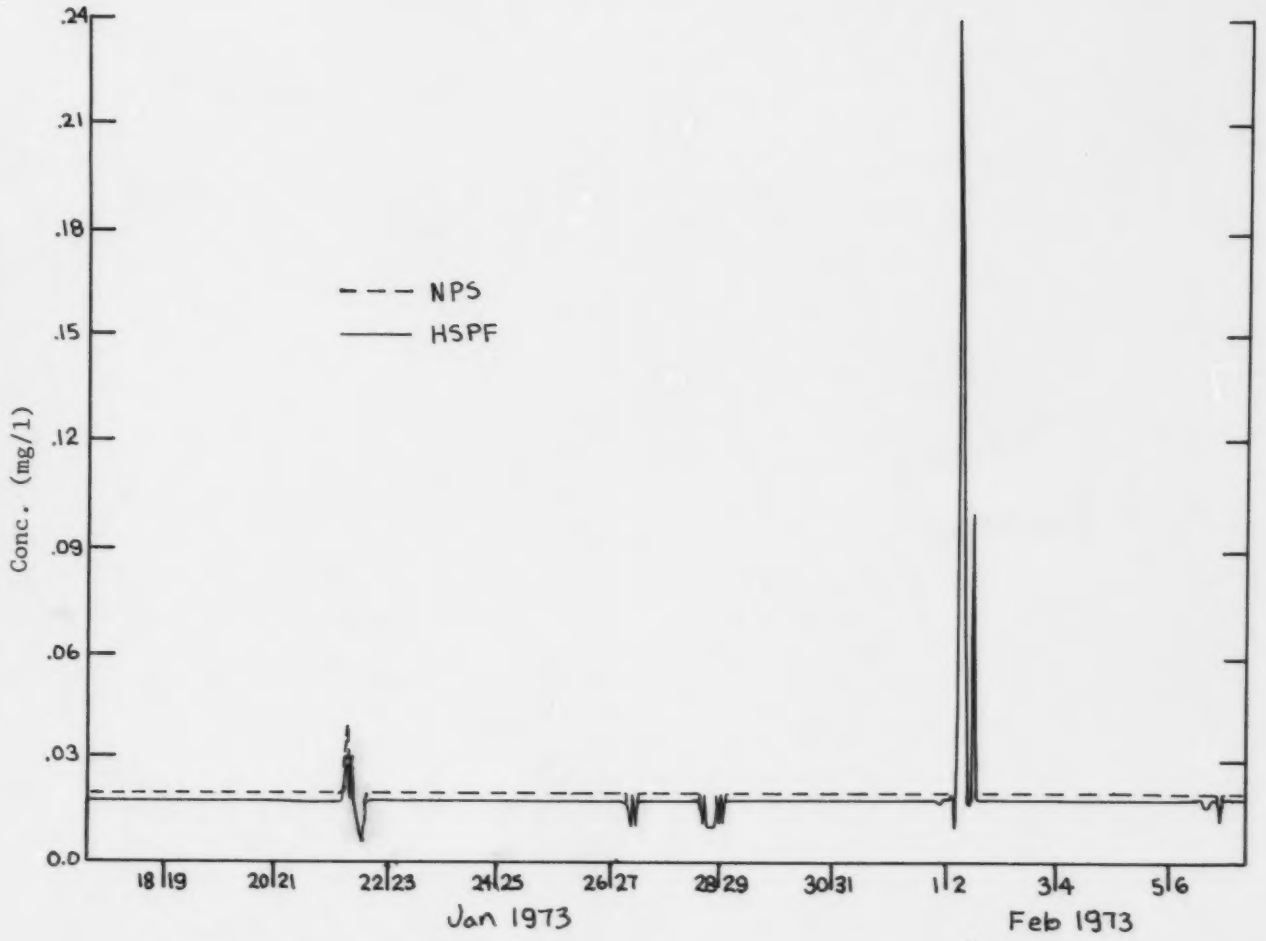


FIGURE 3 SIMULATED CONCENTRATION OF PO4 IN OUTFLOW FROM SUBBA N 4 (OCCOQUAN)

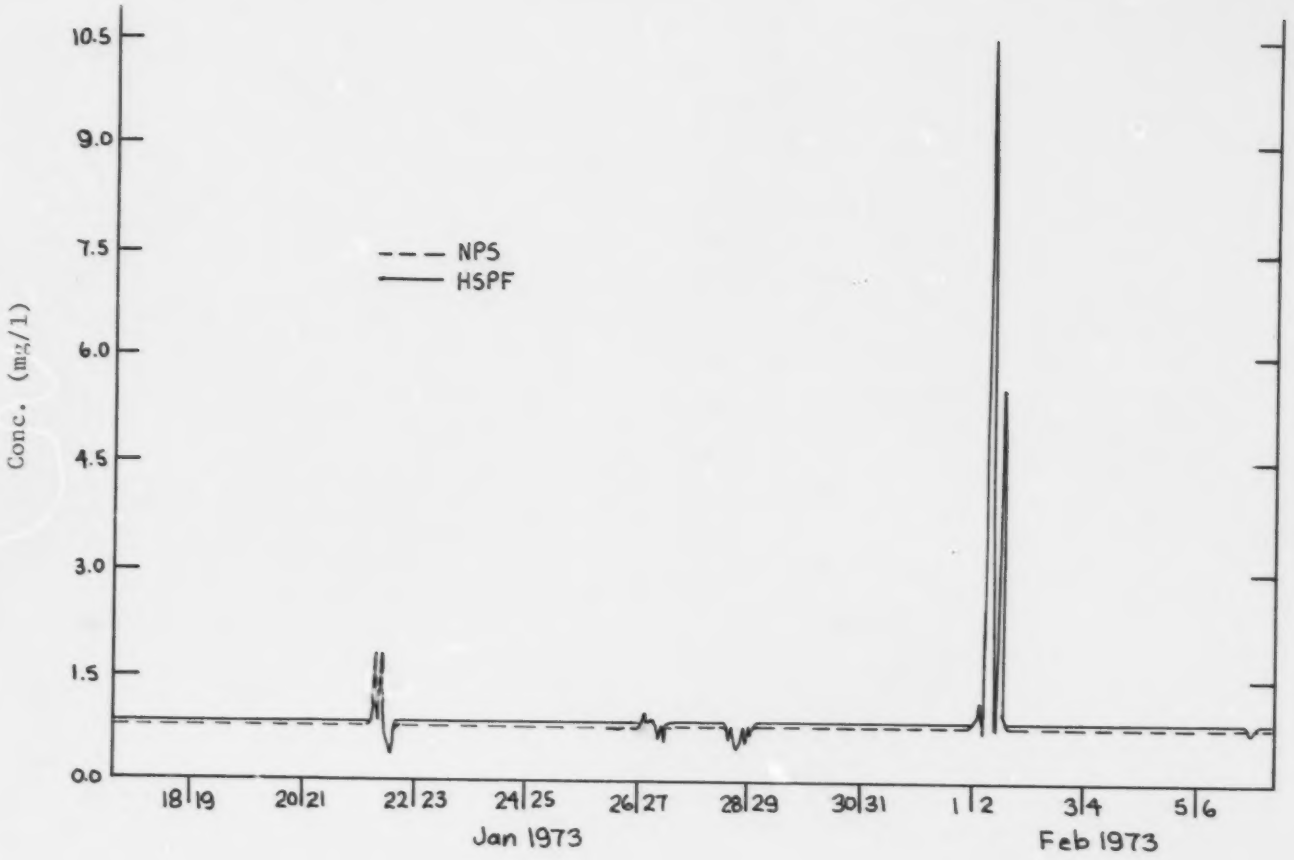


FIGURE 4 SIMULATED CONCENTRATION OF ORGANIC N IN OUTFLOW FROM SUBBASIN 4 (OCCOQUAN)

those in subbasin 5 by a reservoir (50) and those in subbasin 7 by two free flowing reaches (65 and 70).

Designing an HSPF input sequence which represented the channel/reservoir system in a manner exactly equivalent to the HSP-QUALITY model presented problems because:

1. There are many parameters and initial values that must be supplied when doing a water quality run, and the names and definitions of some have changed between HSP-QUALITY and HSPF.

2. HSP-QUALITY represents every reach (including reservoirs) with a trapezoidal cross section. Quantities such as benthal releases are computed using the "bottom area" (length times bottom width). On the other hand, HSPF makes no assumptions about the nature of the cross section and computes benthal releases using an area equal to the surface area. This makes it impossible to get identical results with the two models. However, by adjustment of appropriate parameters, the model outputs can usually be made very similar.

The method used to test the RCHRES module was basically similar to that used to check the land segment simulations:

1. When staff at the NVPDC did the HSP-QUALITY runs, the model wrote to disc the simulated flow rates and constituent concentrations for each reach, on a continuous basis with an hourly time step. These data were transferred to our HP3000 system and were, thus, available for comparison with the corresponding HSPF outputs.

2. The HSPF model was set up to also write its output for each RCHRES to disc (in the Time Series Store).

3. The outputs were compared by plotting them together, and by checking the printed output produced by both models.

4. As before, we could usually identify a problem by observing the nature of the differences between pairs of plotted time series. Usually, it was some value in the user's Control Input which needed adjustment; the problems involved in setting up exactly equivalent inputs have already been discussed. However, this testing work did uncover some bugs in the code and one large discrepancy attributable to a difference in "model convention" (discussed later).

Typical results of this work are shown in Figures 5 thorugh 12. Figure 5 shows that, again, excellent agreement between the hydrologic outputs from the two models was obtained. The simulated water temperatures (Figure 6) were also very similar. Figure 7 has been included to illustrate how the plots were used in some cases to trace bugs in the code. We found that the simulated DO levels agreed well, except that HSPF never permitted the concentration to rise above 12.5 mg/l. An investigation quickly revealed that the maximum allowable concentration was correctly set at the start of the run, to 25% supersaturation, but it was not being updated as the run progressed, in response to changes in water temperature. The bug was easily removed.

The simulation of phytoplankton (Figure 8) was not as easy to reconcile. During October 1973, HSP-QUALITY simulated practically zero growth in RCHRES 50, with the population in the reservoir declining steadily as a result of sinking, respiration, and death of the algae. On the other hand, HSPF simulated very substantial growth in the populaton, until the nutrient supply was exhausted about the middle of the month (Figure 9). Note that

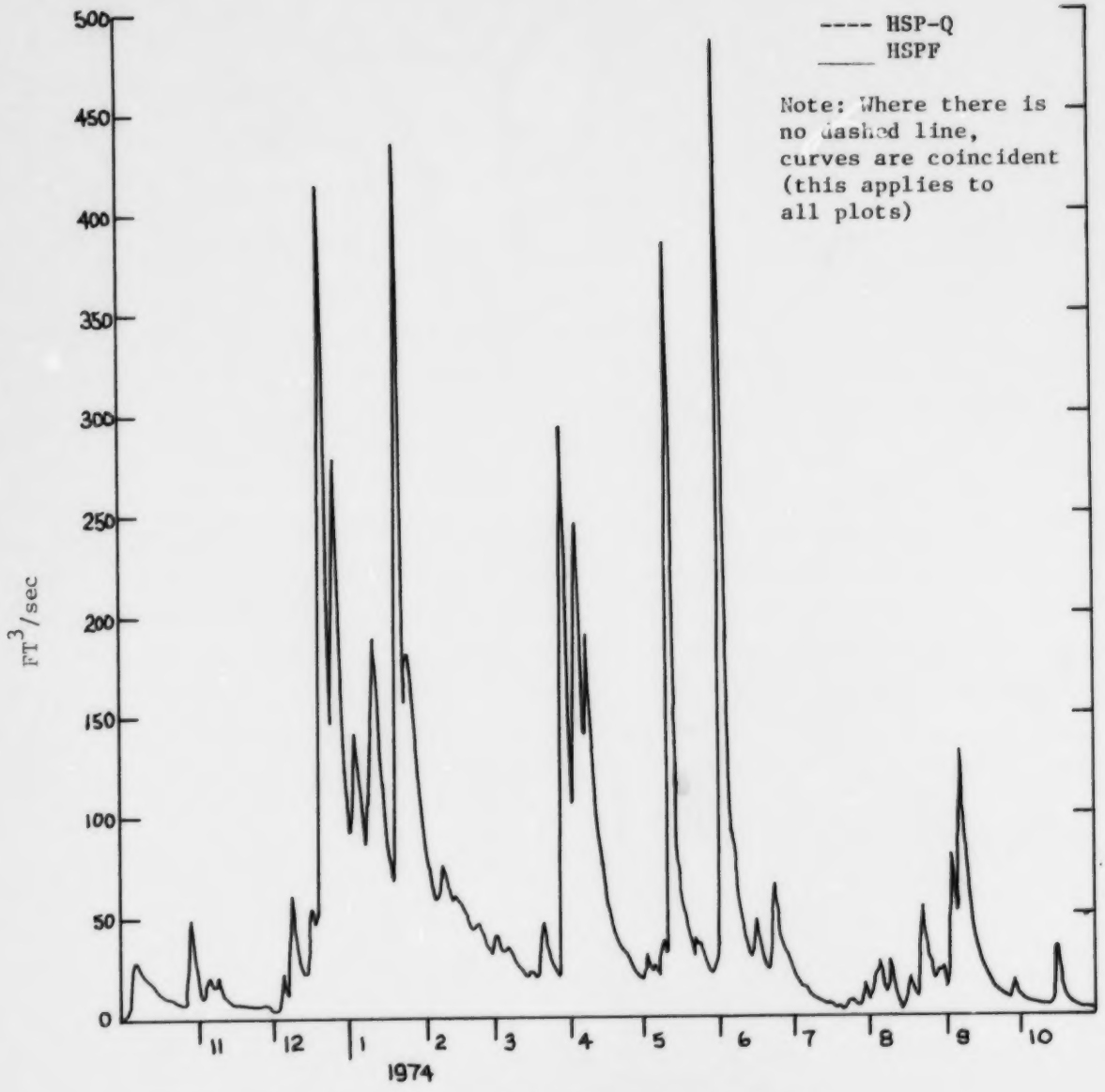


FIGURE 5 SIMULATED OUTFLOW FROM REACH 50 (OCCOQUAN)

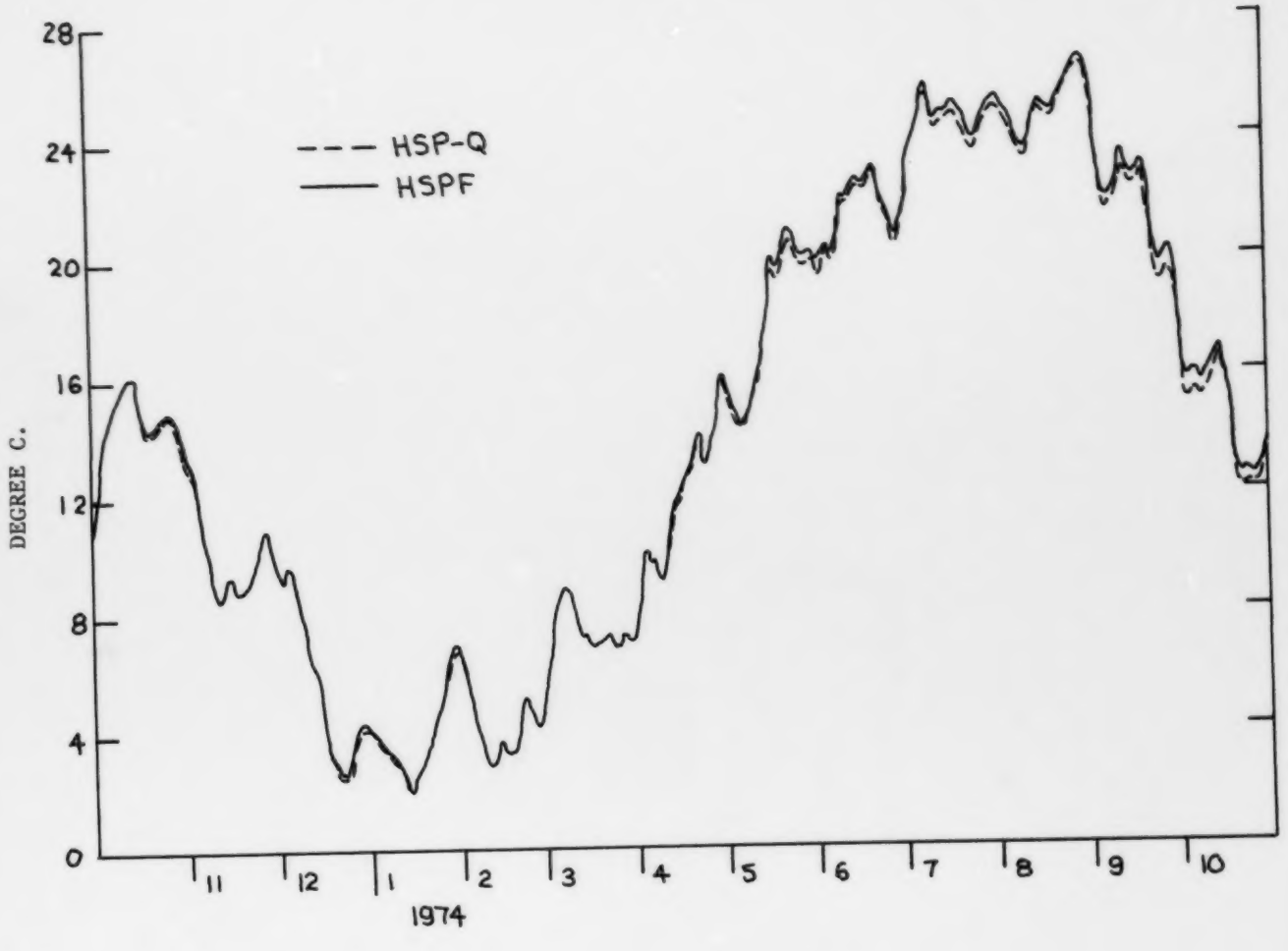


FIGURE 6 SIMULATED TEMPERATURE IN REACH 50 (OCCOQUAN)

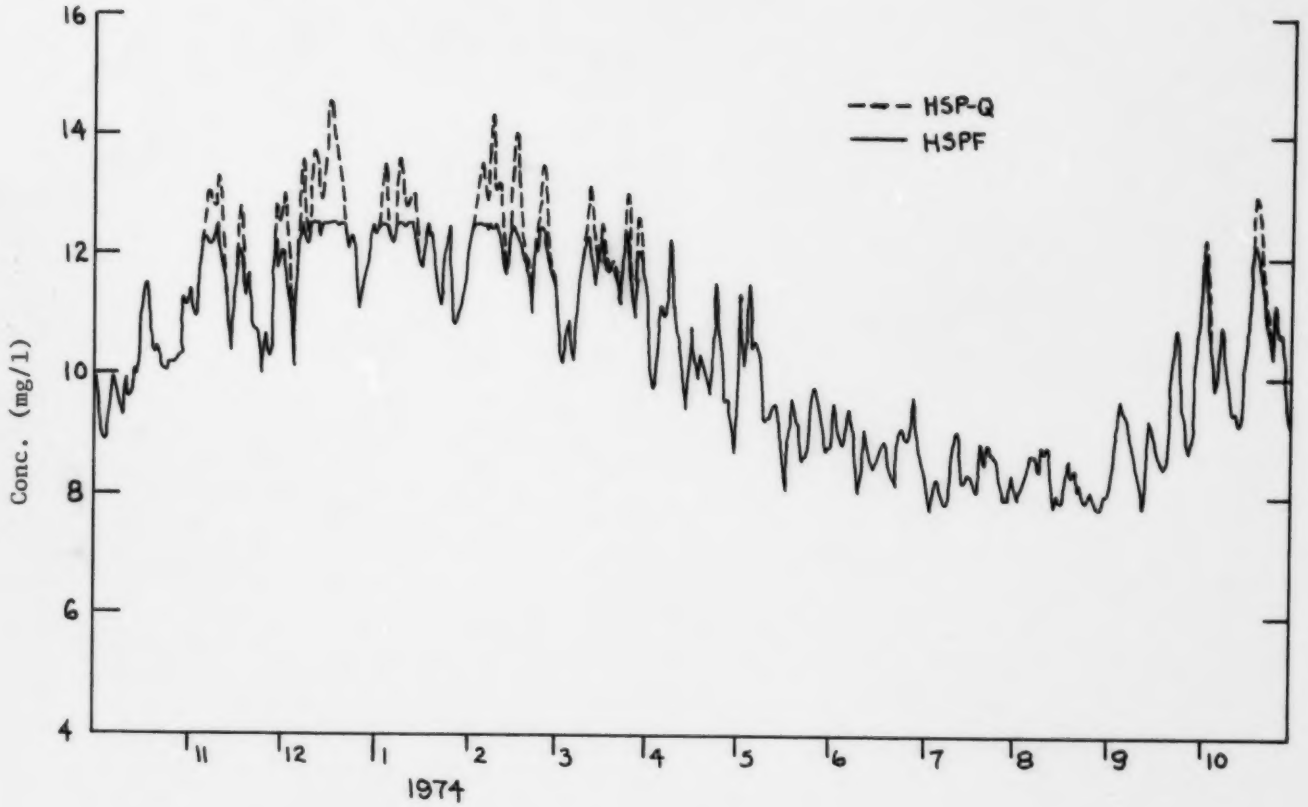


FIGURE 7 SIMULATED CONCENTRATION OF DO IN REACH 40 (OCCOQUAN) - PRELIMINARY RUN

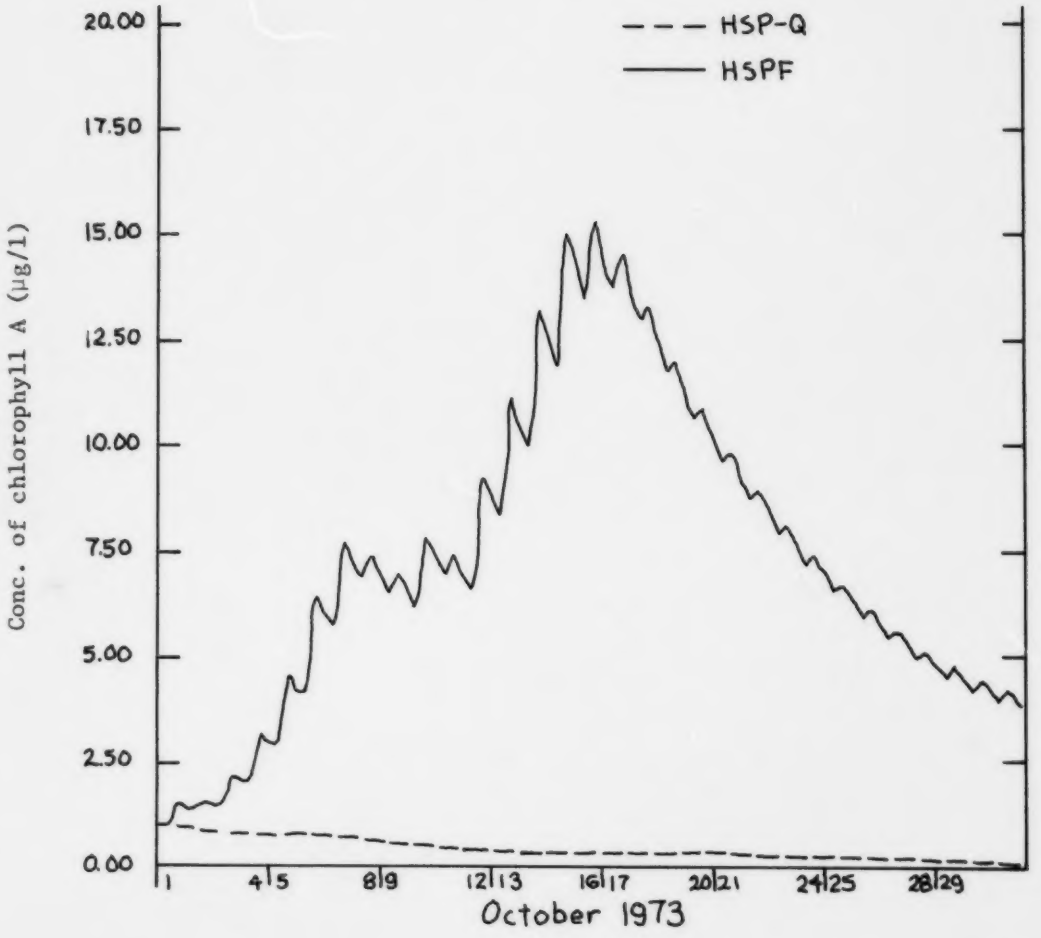


FIGURE 8 SIMULATED CONCENTRATION OF PHYTOPLANKTON IN REACH 50 (OCCOQUAN)

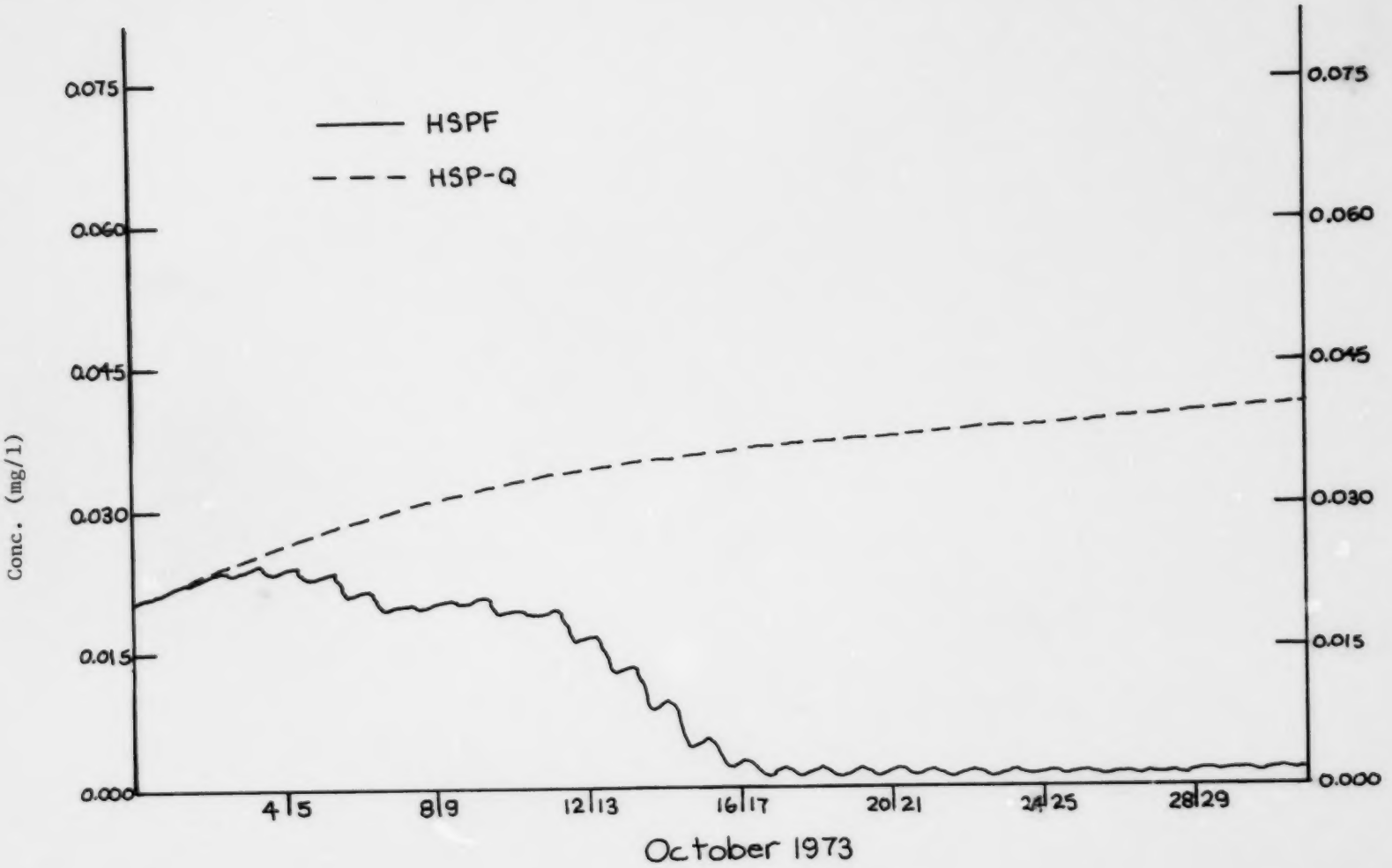


FIGURE 9 SIMULATED CONCENTRATION OF PO4 IN REACH 50 (OCCOQUAN)

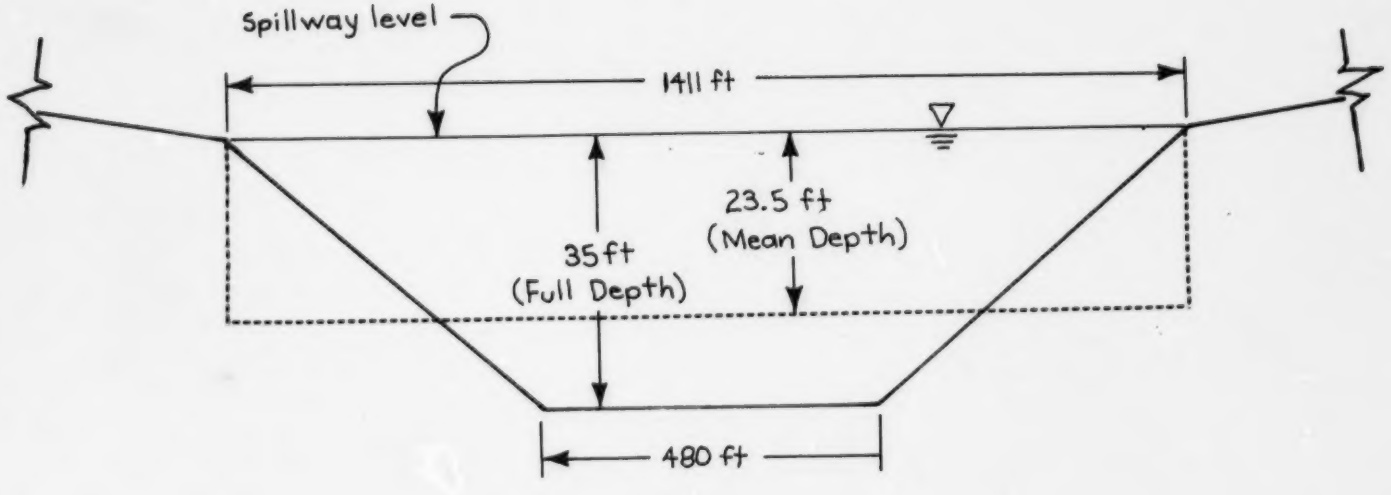


FIGURE 10 CROSS SECTION FOR REACH 50 (RESERVOIR)

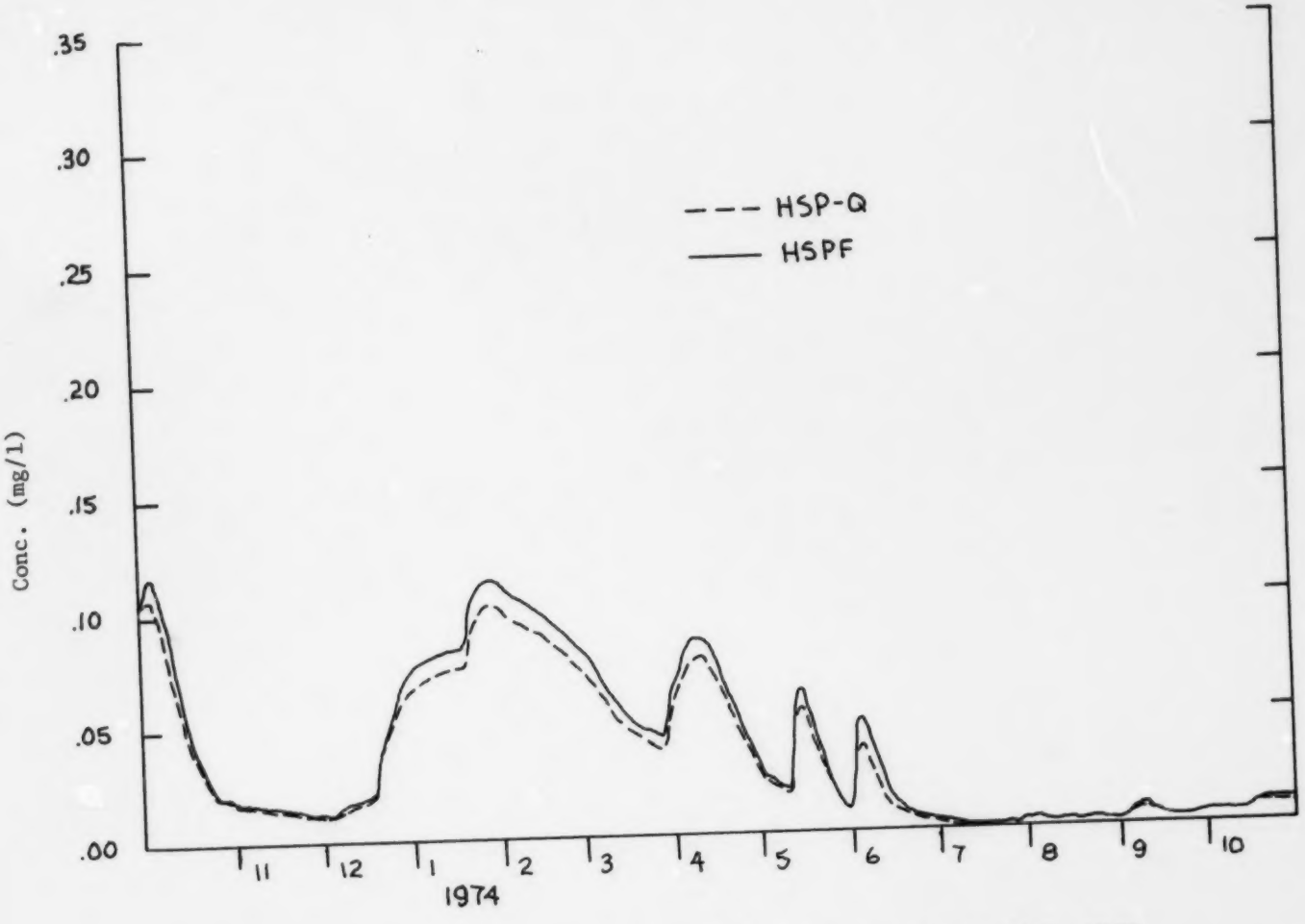


FIGURE 11 SIMULATED AMMONIA CONCENTRATION IN REACH 50 (OCCOQUAN), WITH ADJUSTED PHYTOPLANKTON GROWTH

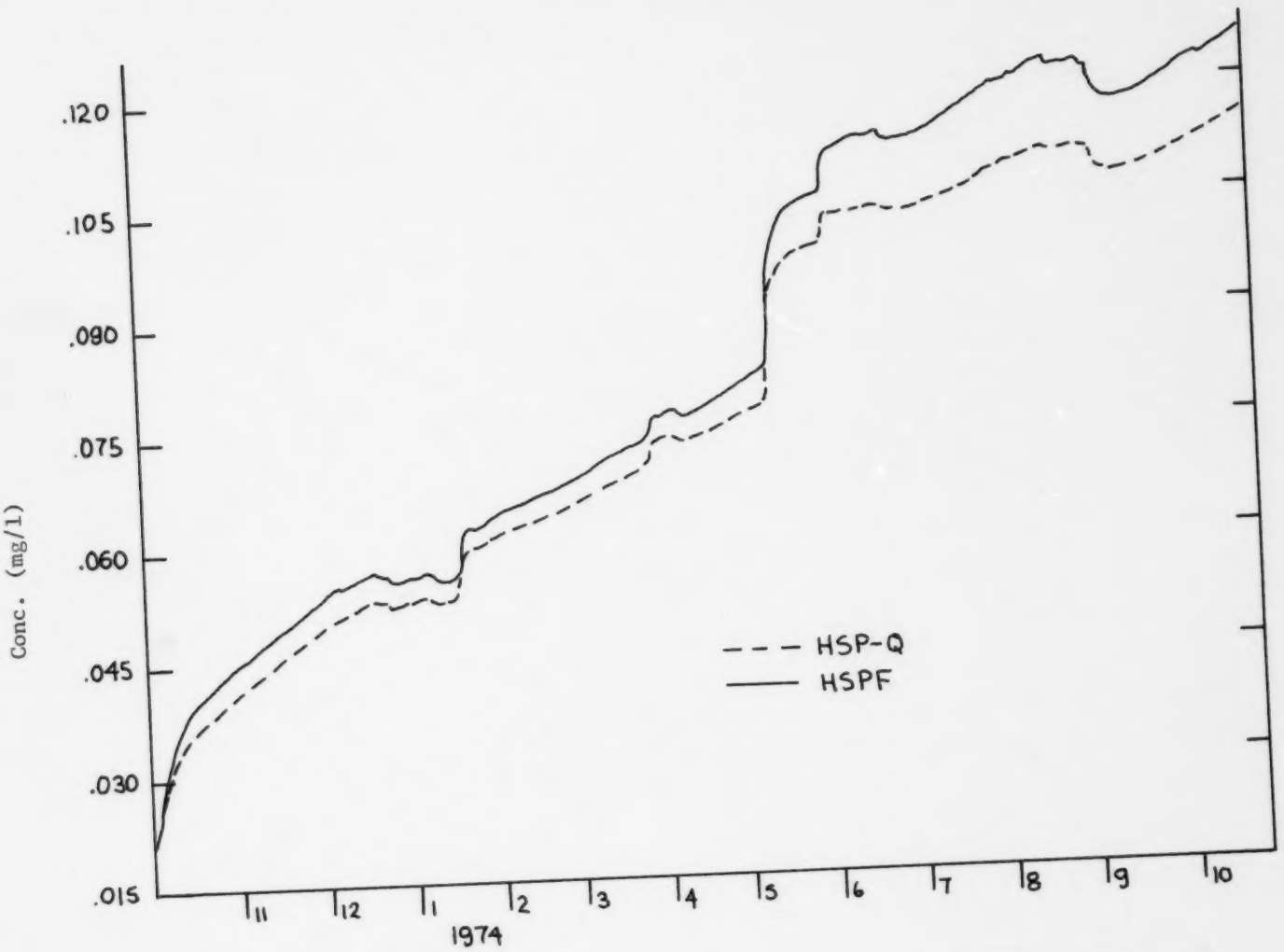


FIGURE 12 SIMULATED CONCENTRATION OF PO4 IN REACH 50 (OCCOQUAN), WITH ADJUSTED PHYTOPLANKTON GROWTH

nitrate was affected in the same way as PO4, although the plot for nitrate is not shown. After the middle of the month a nutrient limited growth condition was reached; the polulation was still declining at the end of the month.

The cause of the phytoplankton discrepancy was difficult to locate. After exhaustive investigations the presence of a difference in the inputs was ruled out, as was the possibiity of a bug in the code. Eventually, we realized that it was due to a "small" difference in the way the two models view the world. The formula used in both models to estimate the light available for phytoplankton growth is:

$$PHYLIT = INLIT \quad e^{-(EXTCO * \frac{Depth}{2})}$$

where INLIT is the light available at the water surface (Langleys/min)

EXTCO is the light extinction coefficient (per foot)

Depth is the water body depth, in feet

Thus, it is assumed that light is extinguished (absorbed) with depth according to an exponential law. To get an estimate of the mean intensity of light in the water body, PHYLIT is estimated using one-half the water body depth. The difference between the two models is the value used for "depth". HSP-QUALITY requires the user to represent all reaches and reservoirs with a uniform trapezoidal cross section and "floodplain" of constant slope (Figure 10). To calculate light extinction, it uses the "full depth" of the water body (35 feet for RCHRES 50, when water is at spillway level). On the other hand, HSPF uses the "mean depth" (cross section area/topwidth); for RCHRES 50, this is only 23.5 feet when the water is at spillway level. Note that the two depths can only be the same for water bodies with vertical walls.

When plugged into the above equation, these two numbers make a tremendous difference. For example, at 10 a.m. on October 1, 1973:

$$\text{HSP-Q:}\quad PHYLIT = 0.582\, e^{-0.284 * 35/2} = 0.0040 \text{ Ly/min}$$

$$\text{HSPF:}\quad PHYLIT = 0.582\, e^{-0.284 * 23.5/2} = 0.021 \text{ Ly/min}$$

In this typical case, a mere difference in the way depth is defined leads to a fivefold difference in light available for phytoplankton growth!

Because we consider the HSPF definition of depth as good as, if not better than, that used in HSP-QUALITY, we do not regard this as a program error. Nevertheless, to permit the best possible comparison of all other aspects of HSPF and HSP-QUALITY output, we proceeded to devise a set of adjusted HSPF input parameters which would give the same growth rate as HSP-QUALITY (this input dataset was called RCHFAKE). To achieve this, we had to change the base extinction coefficient and the Michaelis-Mentan light limited growth parameter. With this done, the HSPF and HSP-QUALITY phytoplankton simulations agreed exactly, confirming that there was no other factor contributing to the problem.

With the above adjustments, great differences in simulation of other constituents that are affected by phytoplankton (potential P, organic N, NH3, DO, NO3 and PO4) were eliminated or reduced. Figure 11 shows the simulation of ammonia in reach 50: the outputs from the two models agree quite well. This agreement is typical of that for most constituents.

There were still some residual problems, however. The worst case was that for PO4 (Figure 12). The situation was carefully investigated. We found no error in the HSPF parameter set or the code. Then we performed a PO4 mass balance calculation on the HSP-QUALITY and HSPF runs. We worked backwards: from the outputs produced by each model, we deduced what the input of PO4 should have been and then compared this with the actual input to reach 50, as reported in the HSPF run (HSP-QUALITY does not report this information). In the case of HSPF the results were consistent: in the case of HSPQ they wre not. Thus, although we were not able to pinpoint the problem, we did conclude that the HSPF PO4 simulation was consistent. The problem probably is that the inflow of PO4 to reach 50 was not exactly the same for the HSPQ and HSPF runs. Data roundoff which incurred when time series were transferred from an HSPQ OSFILE to an HSPF TSS (discussed earlier), could have been the cause.

There was another feature of Figure 12 which concerned us. The difference between HSPF and HSPQ output appears constant from November 1973 through May 1, 1974. But during May 1974 it increases and then again holds constant. This feature was also present in the simulations of NO3 and DO. We were not able to find a definite reason for this but, again, concluded that it was probably due to the two models not being supplied with identical input time series. Note again that the continuity check for PO4 indicated no problem in the HSPF simulation.

Summary

As a result of this work, we concluded that the following parts of the HSPF code had been adequately tested:

SECTION	COMMENTS
PERLND MODULE	
PWATER	with NBLKS=1, DELT=15 minutes
SEDMNT	

PWTGAS
PQUAL

IMPLND MODULE
IWATER with DELT=15 min
SOLIDS
IWTGAS
IQUAL

RCHRES MODULE
HYDR
ADCALC
HTRCH
OXRX
NUTRX
PLANK only phytoplankton was simulated; no zooplankton or benthic algae.

5.4 TESTS ON DATA FROM THE MICHIGAN STATE UNIVERSITY WATERSHED (P6)

Introduction

When this model testing program was devised, we realized that the data obtained for the Occoquan Basin would not suffice to exercise all the simulation algorithms in HSPF. In particular, no snow accumulation and melt simulation was done on the Occoquan, nor were the detailed pesticide and nutrient simulation capabilities of the ARM Model applied there. Thus, it was decided also to use data from P6 watershed in East Lansing, MIchigan. P6 is one of two watersheds in a data gathering program carried on by Michigan State University under EPA sponsorship (Figure 13). It was one of the watersheds used to test the ARM Model. The data collection program, the watershed characteristics and the ARM Model test results have been described

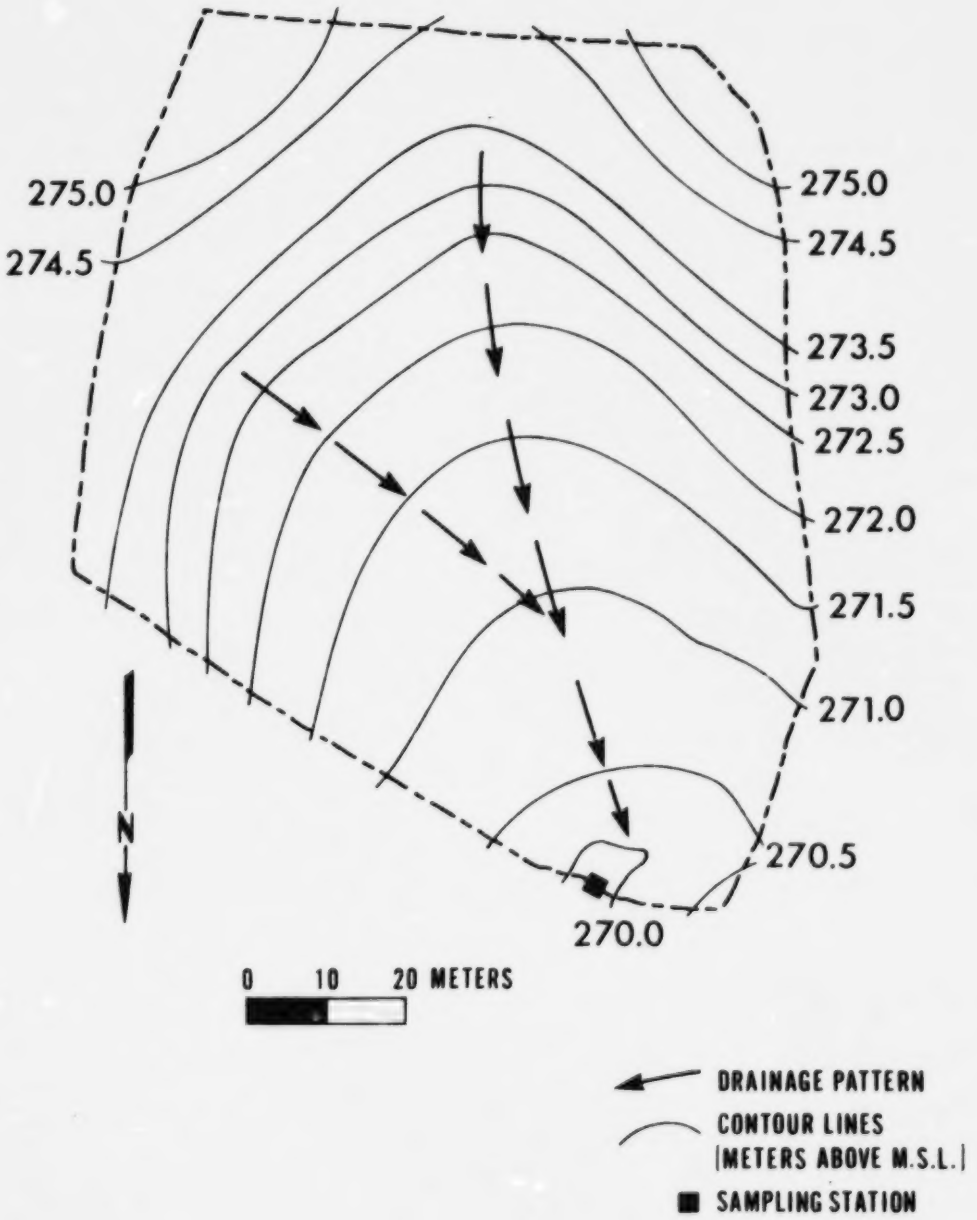


FIGURE 13 P6 Watershed, East Lansing, Michigan (0.8 ha)

in two EPA publications (Donigian and Crawford, 1976 a, and Donigian et. al., 1977).

The P6 watershed is small (0.8 ha) and agricultural. Thus, for simulation using ARM or HSPF, none of it was considered impervious and no channel system was modeled. To make an HSPF simulation which was equivalent to an ARM run, the watershed was represented by a single, pervious land segment. It follows that this test program only exercised code in the PERLND module; in particular, those sections of PERLND which incorporate the features of the ARM Model:

Section SNOW - simulates accumulation and removal of a snowpack

Section PWATER - simulates the water budget in a pervious land-segment

Section SEDMNT - simulates the detachment and washoff of sediment

Section PSTEMP - simulates soil temperature

Section PEST - simulates pesticide behavior

Section NITR - simulates nitrogen behavior

Section PHOS - simulates phosphorus behavior

Section TRACER - simulates a tracer (conservative) substance

Method

One useful feature of the HSPF-system is that the various sections of an application module can be selectively activated. Thus, with the PERLND module (Figure 14), you can start by running section SNOW only. When you are satisfied with its behavior you can also turn on Section PWATER and check it out. This permits "incremental" calibration or testing of the module which is a useful feature, because you do not have to waste time simulating a section until all those sections which affect it are checked out. We used this technique; the various sections of PERLND were tested in "left-to-right" sequence (Figure 14).

First, the meteorological input time series (precip., PET, Temp., etc.) for P6 were converted to HSPF format and read into a TSS. Then, for each section tested:

1. The ARM Model input parameters and initial conditions, as well as the corresponding output, were obtained. In most cases, we were able to make use of the printouts from runs made when ARM was being tested. However, we sometimes found the (monthly) output summaries provided too little information to track down the cause of an HSPF/ARM difference, and we had to make special short ARM runs and print at a daily, or even hourly, interval.

2. HSPF was run with a corresponding input stream. Monthly summaries, as well as detailed information for selected events, were displayed.

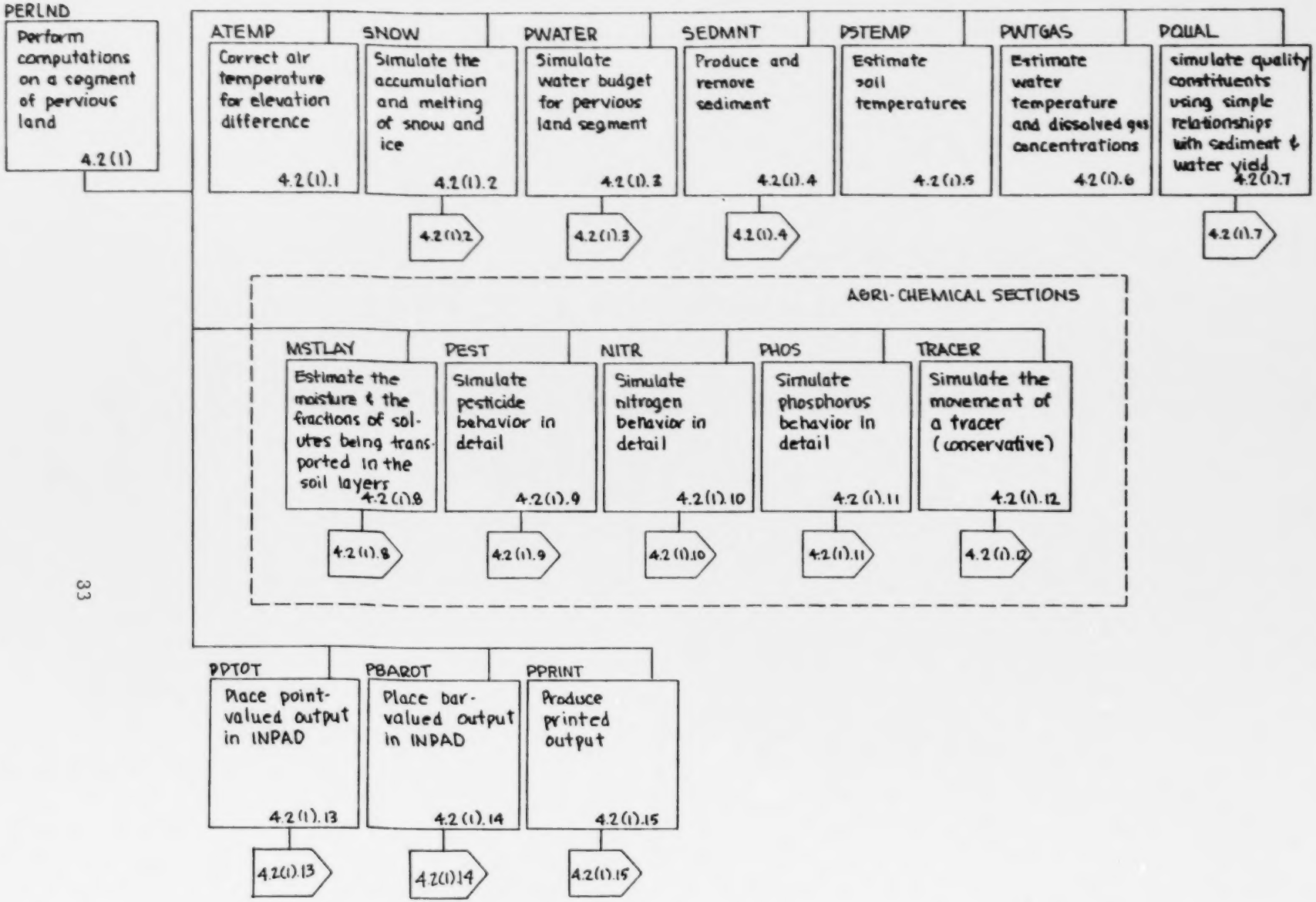


FIGURE 14 STRUCTURE CHART OF THE PERVIOUS LAND-SEGMENT APPLICATION MODULE

3. The results were compared and the causes of observed differences were found. This step took more time than it did with the Occoquan data because we could not produce the HSPF vs. ARM plots by machine. The ARM results were on printouts, not on disc, so they had to be manually plotted. A master copy of each plot was prepared, with the ARM output on it, and the output from each succeeding HSPF run was plotted on a copy of this master.

4. Changes were made to the HSPF input or code and then the process was repeated.

Simulation of Snow Accumulation and Melt (Section SNOW)

Figure 15 shows the snowpack simulations produced by ARM and HSPF for Nov/Dec 1974. In general, the agreement is good, but there are significant differences. These were investigated. When precipitation occurred on November 5, the ARM model interpolated (from daily max/min values) an air temperature slightly below that required to form snow (TSNOW); hence the simulation "produced" snow, which melted by November 9. However, the interpolation algorithm used in HSPF gave a slightly higher temperature and, thus, the pecipitation was simulated as rain, not snow. In such a marginal situation, the true air temperature was probably significantly different from the values used by both models, so had about the same probability of being right (or wrong).

Most of the other discrepancies are attributable to the fact that CLDF (a cloud cover factor) is updated irregularly in the ARM model, instead of each time step, as in HSPF. This affects the simulated radiation energy balance because ARM can simulate a high rate of longwave energy loss, corresponding to clear sky conditions, during which it also simulates snowfall, a coincidence which appears physically impossible. This problem accounts for the differences in model behavior on November 29 and December 15, 23, and

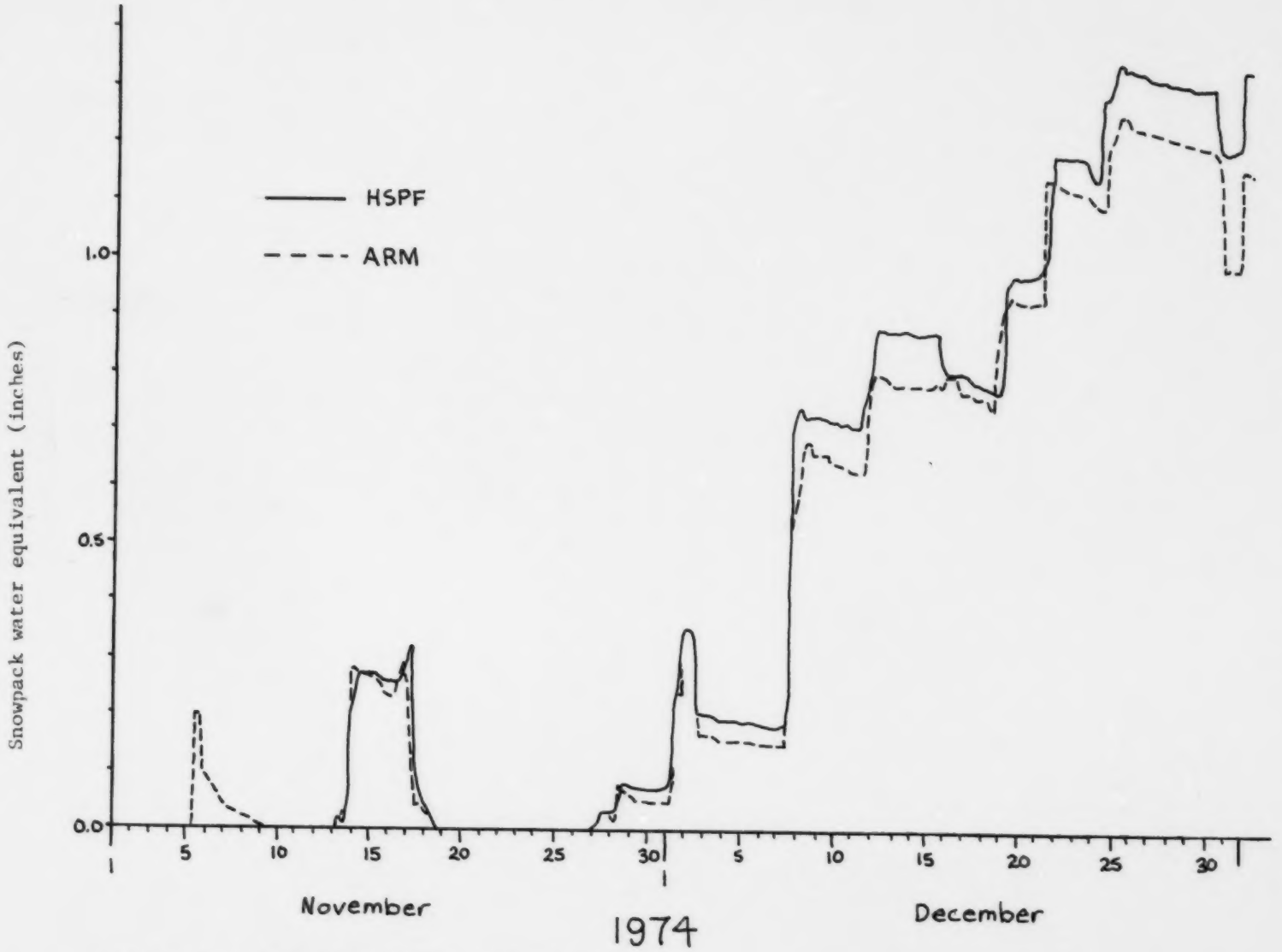


FIGURE 15 SIMULATED SNOWPACK, P6 WATERSHED

30, which are cumulative in effect. We believe that the HSPF code more closely represents the natural process.

Simulation of Water Budget and Sediment Yield (Sections PWATER and SEDMNT)

Sections PWATER and SEDMNT had been checked out when performing tests on the Occoquan basin data. However, there were two substantial differences between those tests and the application to watershed P6:

1. On the Occoquan, the time step was 15 mins.; on P6 it was 5 mins.

2. The ARM Model subdivides a land-segment into 5 "areal source-zones" (Donigian and Crawford, 1976 a); the HSP and NPS models do not use this feature--they use only one areal source-zone. In HSPF, the user can set the number of source-zones, called "blocks", to any number from 1 through 5. The value selected does affect the hydrologic response to some extent. Thus, when using HSPF to replicate the NPS model simulation of the Occoquan, we set NBLKS=1. When reproducing the ARM Model simulation of P6, we set it to 5.

The tests on the Occoquan and P6 data, therefore, tested different aspects of model sections PWATER and SEDMNT.

As with the testing described earlier, most of the work in reconciling differences betwen ARM and HSPF output did not result in updates to the HSPF code, but in changes to the HSPF input stream to make it exactly equivalent to the ARM input. As before, this work was not easy because some of the differences between HSPF and ARM inputs are quite subtle. For example, ARM allows the user to specify a set of 12 monthly values for the fraction of ground which is covered (COVPMO), but it only requires a single value for the interception storage capacity (EXPM). This is actually the maximum storage capacity, corresponding to maximum cover; the program automatically

adjusts the interception storage capacity continuously by prorating it according to the amount of cover. It is easy for the user to forget that this is happening. In HSPF, on the other hand, the user must explicitly specify whether cover and/or interception storage capacity are to vary through the year. If either quantity does vary, he must supply 12 monthly values for it. There is no automatic connection between the seasonal variations in ground cover and interception storage capacity. Our own misunderstanding of this difference between the models costs several days effort.

The precipitation and E-T simulated by the two models are shown in Figure 16. Although the meteorological input time series were identical, the precipitation values for November and December differ because the two models did not always agree on the assignment of precipitation as snow or rain. When it is treated as snow the "snow catch factor" (1.4) is applied to recorded precipitation to estimate actual snowfall. Hence the small differences in those months.

The E-T simulated by both models agrees closely, indicating that the hydrologic response of the two is very similar. This is confirmed in Figure 17, which indicates that the monthly values of simulated runoff plus groundwater recharge are close, with the exception of November. Figure 18 shows the components of runoff; surface runoff and interflow. Again, agreement is close except in the months of November and December. The anomaly in these winter months was investigated and found to be due to a convention implemented in the HSPF code, whereby snowmelt was accumulated until it reached a value of 0.01 inches, and was then suddenly released onto the land surface. ARM released the melt water gradually, as melt took place. This seemingly small difference between the models was responsible for the very different simulated outflows when snowmelt occurred; HSPF produced more runoff because it released the melt-water in sudden "bursts" which did not infiltrate and too much ran off. The problem was corrected by modifying the

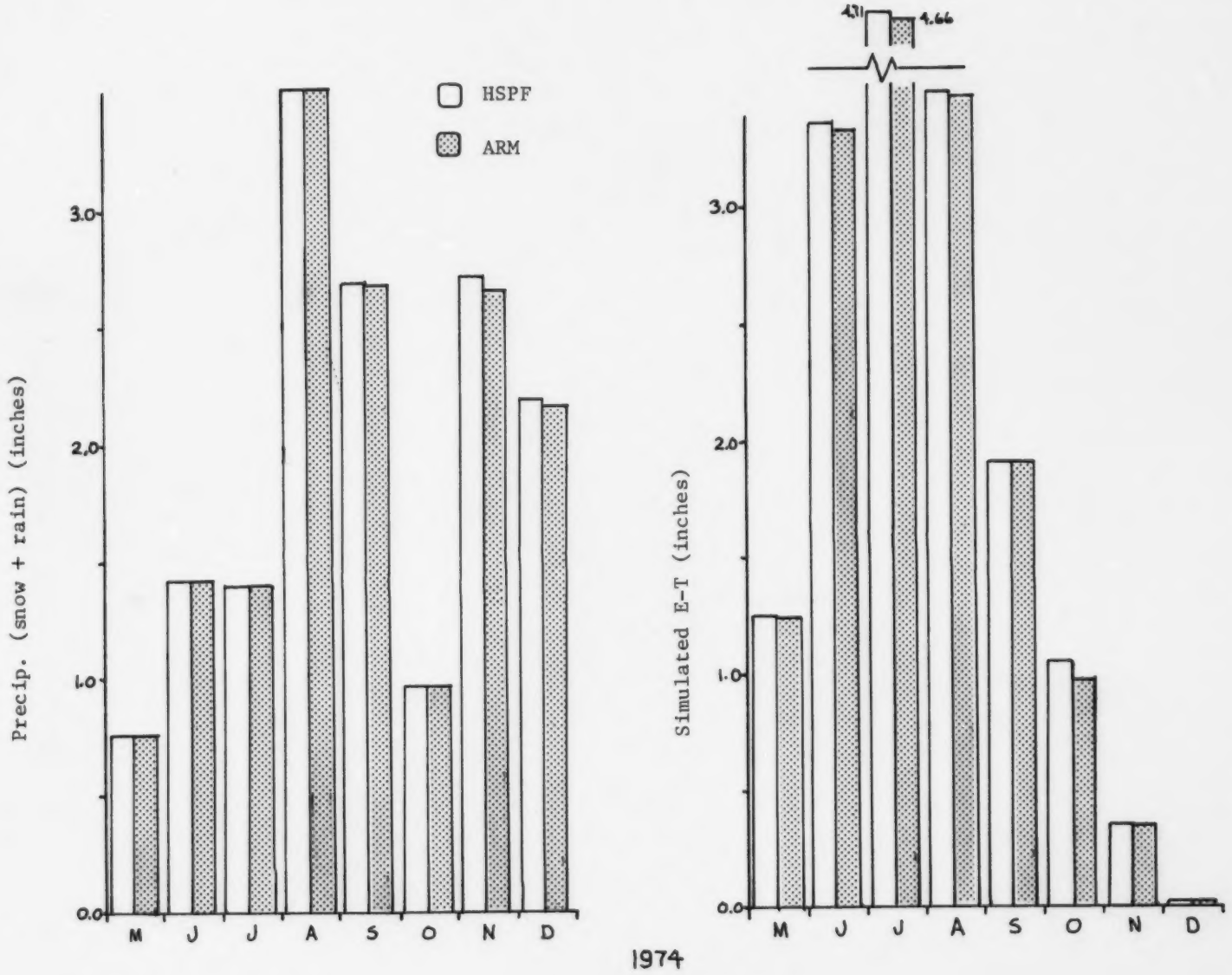


FIGURE 16 PRECIPITATION AND SIMULATED E-T, P6 WATERSHED

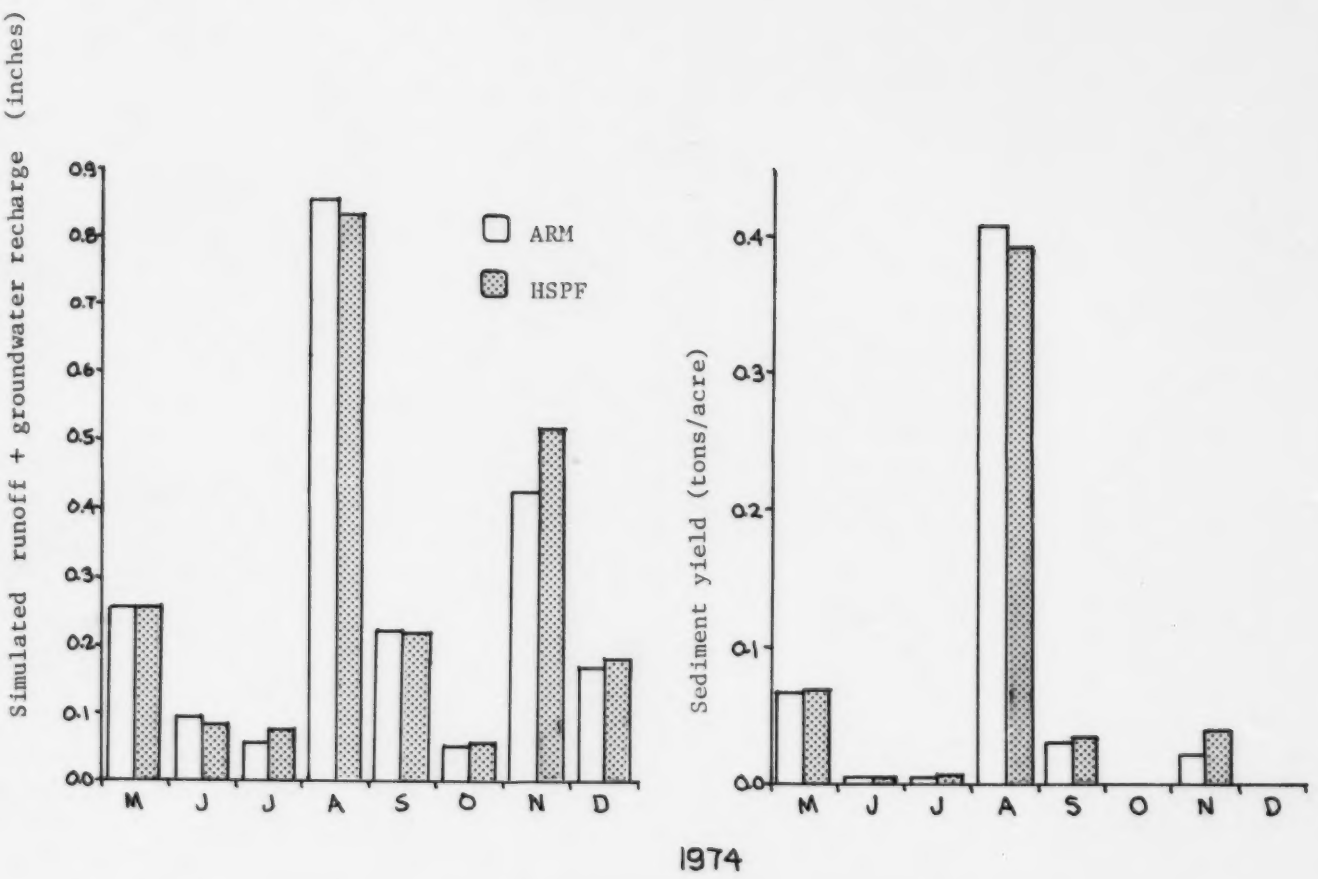


FIGURE 17 SIMULATED RUNOFF AND SEDIMENT YIELD, P6 WATERSHED

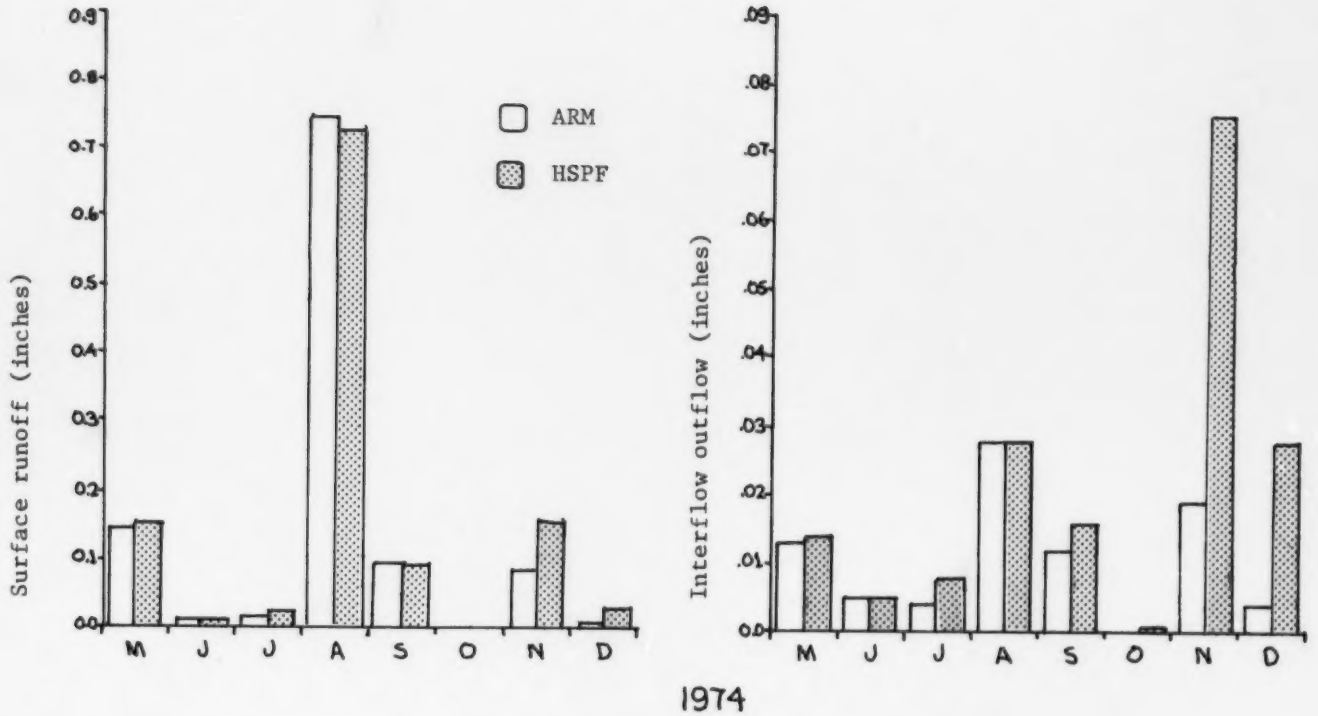


FIGURE 18 SIMULATED SURFACE RUNOFF AND INTERFLOW OUTFLOW, P6 WATERSHED

HSPF code to release melted snow more gradually, which eliminated the large November and December differences in Figures 17 and 18. The graph of monthly sediment yield (Figure 17), shows generally close agreement between the two models. The discrepancy in the values for November was fixed by the measure described above.

The simulated runoff and sediment yield for two storm events, those of August 13 and 27, 1974, are shown in Figures 19 and 20. Agreement is very good, except for small discrepancies in the first peak of each event. On August 13, HSPF gave a lower value, on August 27 a higher value. The difference is probably due to the two models having slightly different moisture in the upper zone (UZS) at the start of each event, but we don't have sufficient printout to prove this.

Simulation of Pesticide Behavior (Section PEST)

The processes which affect agricultural chemicals, as simulated in the ARM and HSPF models, fall into two categories: advection and reaction. Advection is the transport of chemicals over the soil surface or through the soil. In our models the land-segment is viewed as having four "layers": surface, upper, lower, and groundwater (Donigian and Crawford, 1976 a; Johanson et. al., 1979). Soluble chemicals are transported by water between these layers, which have storages associated with them. Also, the soluble chemical moves from one or more of these storages to the stream channel (with surface runoff, interflow or groundwater outflow) or to deep groundwater. Insoluble chemicals can only be washed to the stream system from the surface layer of the soil. In HSPF, advection of soluble chemicals is governed by section MSTLAY of the PERLND module. It uses the results produced in the water budget calculations (Section PWATER) to estimate the fraction of stored soluble chemical that will leave each storage along each flow path, in each time step.

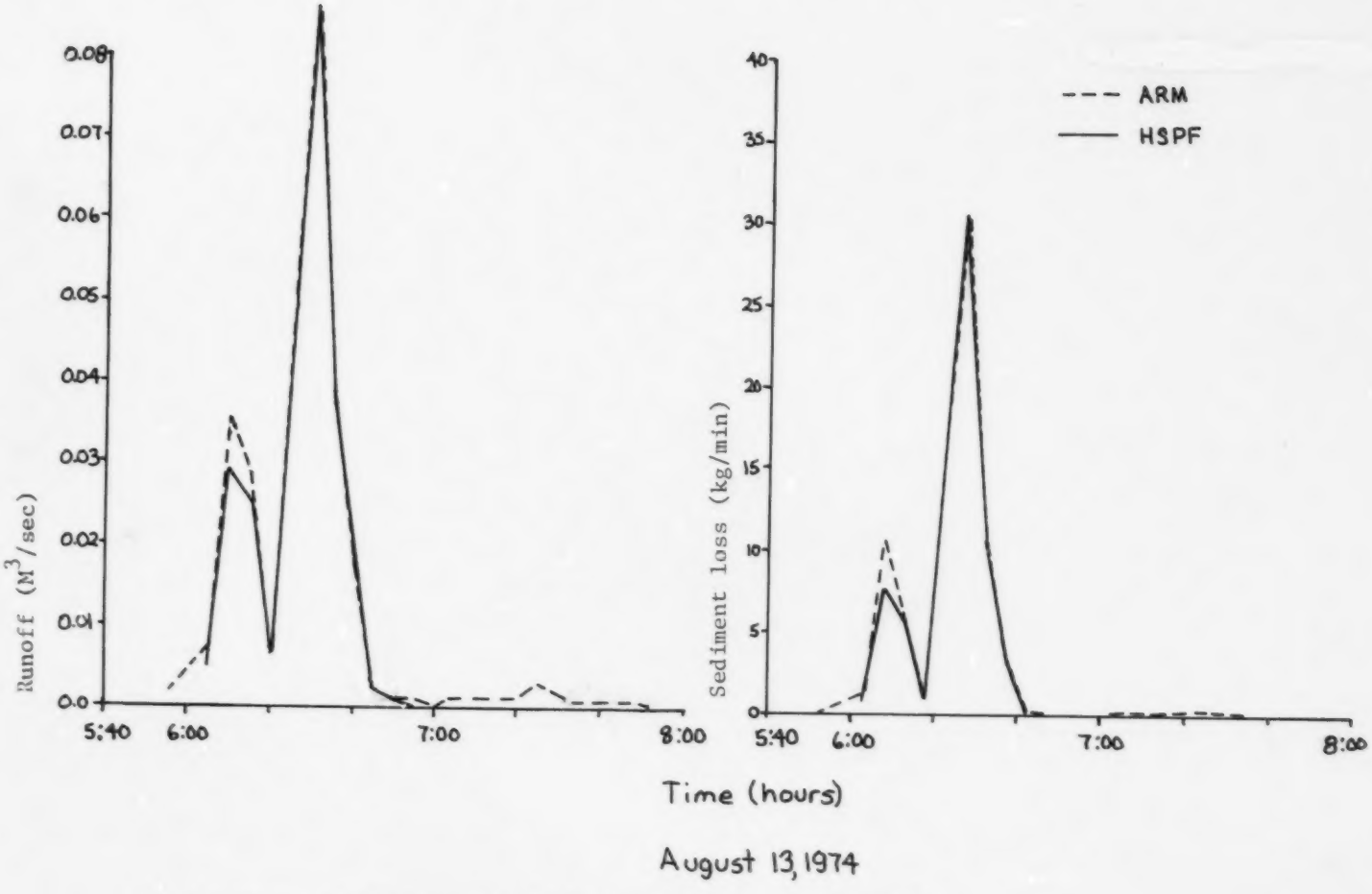


FIGURE 19 SIMULATED RUNOFF AND SEDIMENT LOSS FOR STORM OF AUGUST 13, 1974 - P6 WATERSHED

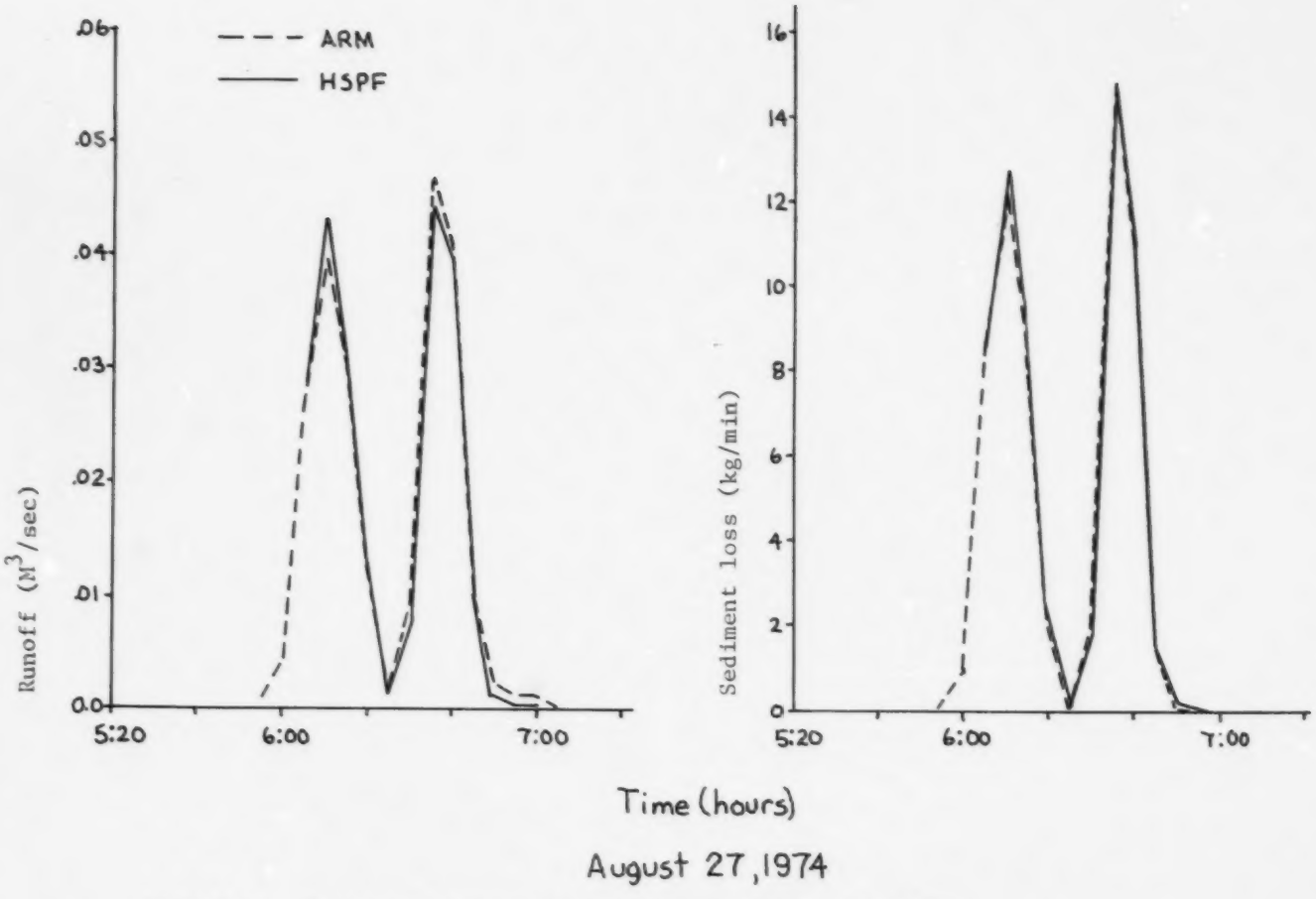


FIGURE 20 SIMULATED RUNOFF AND SEDIMENT LOSS FOR STORM OF AUGUST 27, 1974 - P6 WATERSHED

"Reaction" refers to the transformations that a chemical undergoes as a result of physico - chemical processes. In ARM and HSPF two processes are considered for pesticides:

1. Adsorption/desorption. This is the movement of ions between the dissolved state and the "adsorption sites" provided by fine sediment particles. ARM and HSPF use a "Freundlich isotherm" (Donigian and Crawford, 1976 a) to simulate the process. Either a single-valued or non-single-valued isotherm may be used. In these tests the latter method was used.

2. Degradation. This term includes volatilization and degradation due to microbial action. It is handled with a first-order equation, using a degradation constant input by the user.

In nature, advection and reaction take place simultaneously and continuously in time and space. In most models, including ARM and HSPF, the processes must be separated and discretized.

In ARM, the sequence of operations for pesticides is:
1. React in the surface layer
2. Advect from the surface layer
3. React in the upper layer
4. Advect from the upper layer

etc.

In each time step, the model first performs reactions, assuming the solution and adsorbed phases of the pesticide reach equilibrium instantaneously. Then it assumes no further reacting takes place, while it simulates advection for the time step.

HSPF also first reacts pesticides and then advects them but performs reactions in all layers before starting with the advection.

For nutrients, the models sequence these operations differently. This will be discussed later. At this stage it suffices to note that the sequencing, although it is only a detail of model construction and not a fundamental consideration, can have a dramatic effect on the results produced. This will be demonstrated later.

The results obtained for pesticide simulation are shown in Figures 21 through 24. The tests covered two pesticides, atrazine and paraquat. Atrazine exists in significant quantities in both the adsorbed and dissolved states but paraquat is so highly adsorbed that it exists and moves almost entirely on sediment.

Figure 21 shows that the simulated storages of atrazine in the surface and upper layers agree quite well, for the two models. Atrazine was applied to the watershed on May 21 (3.52 lb/acre) and November 8 (2.68 lb/ac). After each application, degradation destroyed 5% per day, so that the storage decreased rapidly. The simulated removal of atrazine (Figure 22) also shows this effect; removal declines rapidly after the time of application.

The apparent difference in atrazine removed on sediment (Figure 22) is not real, because the output from the ARM run was only reported to 3 decimal places. The higher total removal simulated by HSPF for May 1974 is probably due to the slightly different way in which the various reaction and advection operations are sequenced and represented in the two models. The higher removal reported by HPSF is consistent with the lower value that it reports for the storage of atrazine at the end of May 1974 (Figure 21).

The removals of paraquat simulated by the two models agree quite closely (Figures 23 and 24). This is quite understandable. Paraquat is so highly

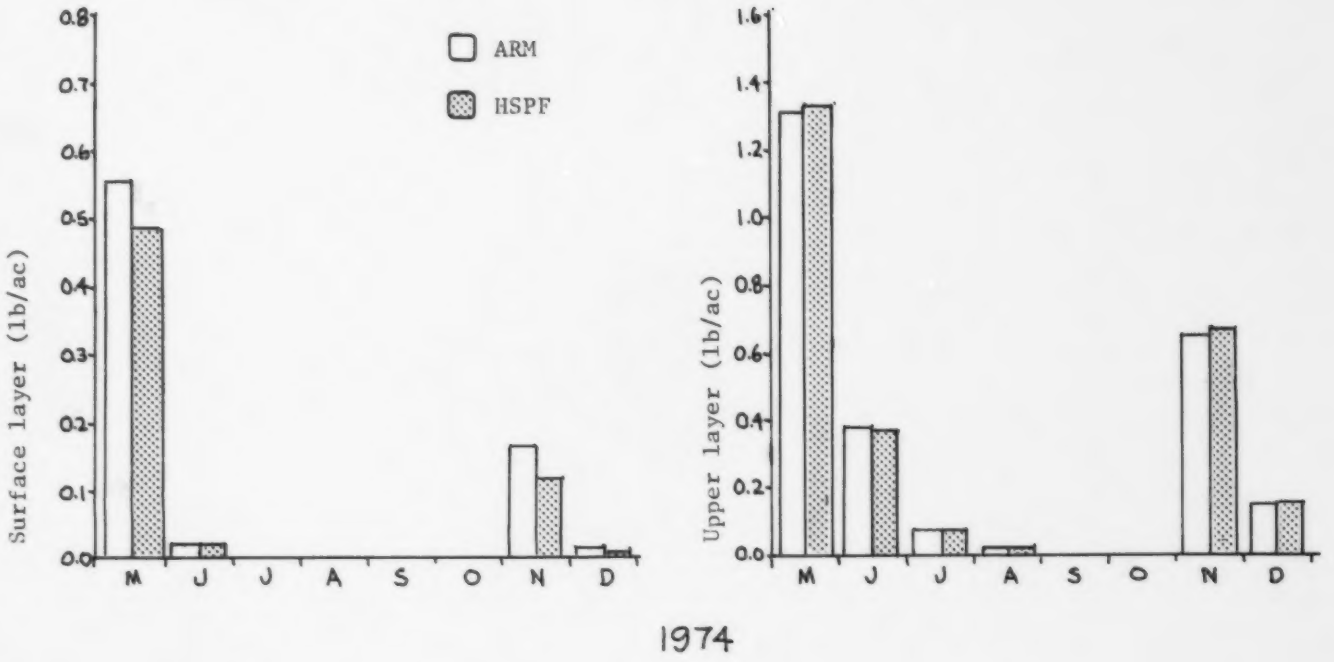


FIGURE 21 SIMULATED STORAGE OF ATRAQINE IN THE SURFACE AND UPPER LAYERS, P6 WATERSHED

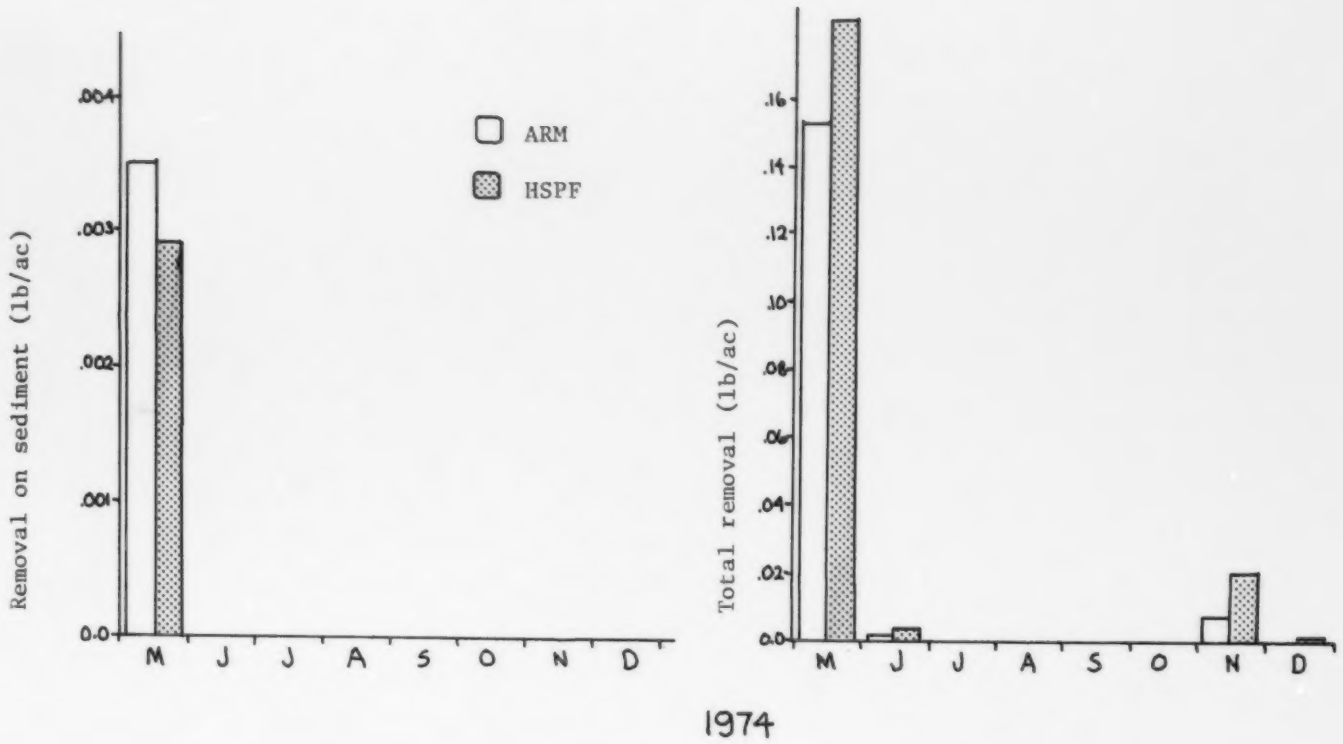


FIGURE 22 SIMULATED REMOVAL OF ATRAQINE - P6 WATERSHED

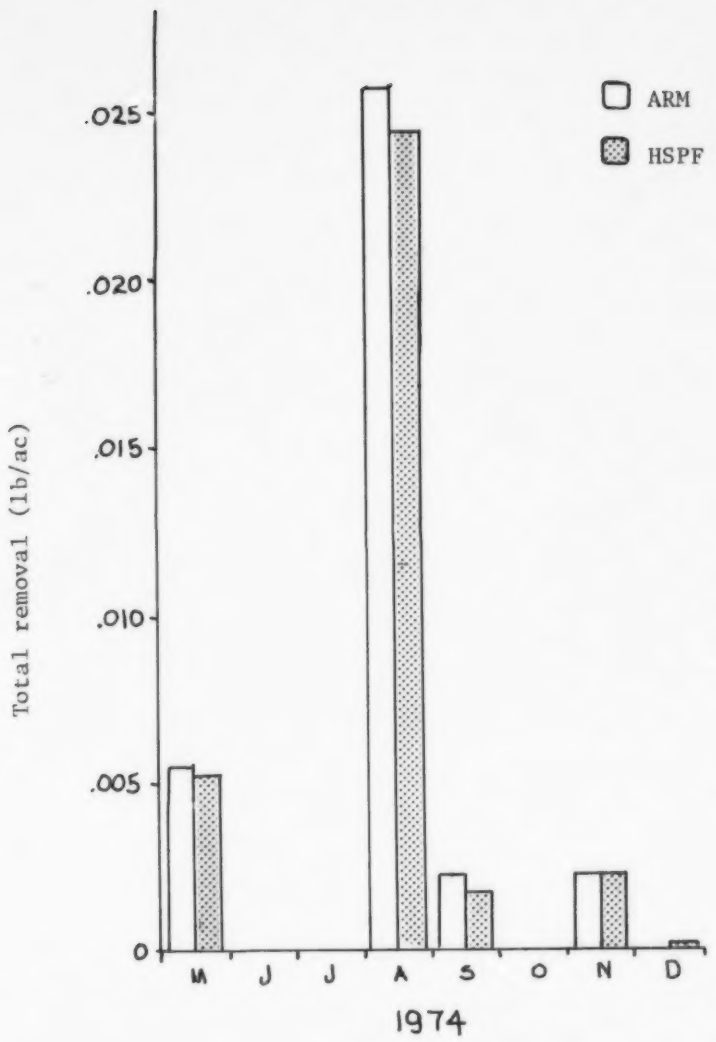


FIGURE 23 SIMULATED REMOVAL OF PARAQUAT - P6 WATERSHED

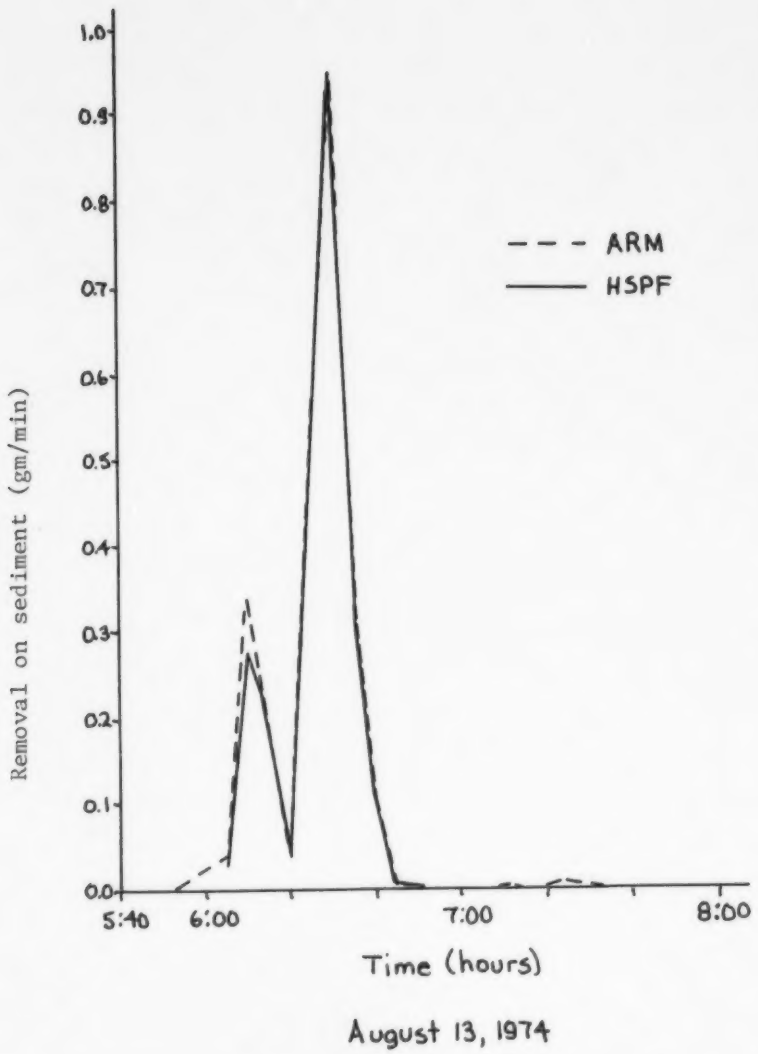


FIGURE 24 SIMULATED REMOVAL OF PARAQUAT ON SEDIMENT - PT WATERSHED

adsorbed, that almost all removal occurs on sediment. Thus, the two simulations must agree about as closely as the corresponding simulation of sediment removal.

When this testing work commenced, HSPF performed all the advection in a land-segment before the reactions were simulated. We found it impossible to closely reproduce the ARM Model results with this arrangement; for example, the atrazine storages at the end of May 1974 were (lb/ac):

	ARM	HSPF
SURFACE LAYER	0.55	0.8
UPPER LAYER	1.35	1.0

Obviously HSPF simulated much less percolation from the surface to the upper layer. We concluded that this could be entirely due to the different sequencing of advection and reaction in the two models. So the HSPF code was altered, to make its sequence coincide as closely as possible with ARM and, as expected, the differences practically disappeared. This result illustrates the point made earlier, that choice of conventions (e.g., advect then react, vs. react then advect) can have a substantial effect on the results produced by a model. The effect could be even larger than that produced by a change in algorithm, such as a switch from the single-valued to non-single-valued Freundlich isotherm.

Simulation of Nutrients (Sections NITR and PHOS)

The introductory comments, made in discussing the simulation of pesticide, are also applicable to nutrients. The principal differences between the

simulation of pesticides and nutrients are:

1. A greater number of chemical species are simulated in the case of nutrients. Figure 25 shows the various forms of nitrogen and phosphorus represented in the ARM and HSPF models, and the associated reactions: nitrite and nitrate are combined; NO2+NO3 is increased by nitrification of dissolved NH4, and decreased by denitrification, plant uptake and, possibly immobilization to the organic form. Ammonia can undergo adsorption and desorption, and the dissolved form can interact with organic N through the ammonification and immobilization reaction paths. Phosphate adsorption and desorption is simulated. The dissolved phosphate can also be affected by plant uptake and interaction with the organic form (mobilization and immobilization).

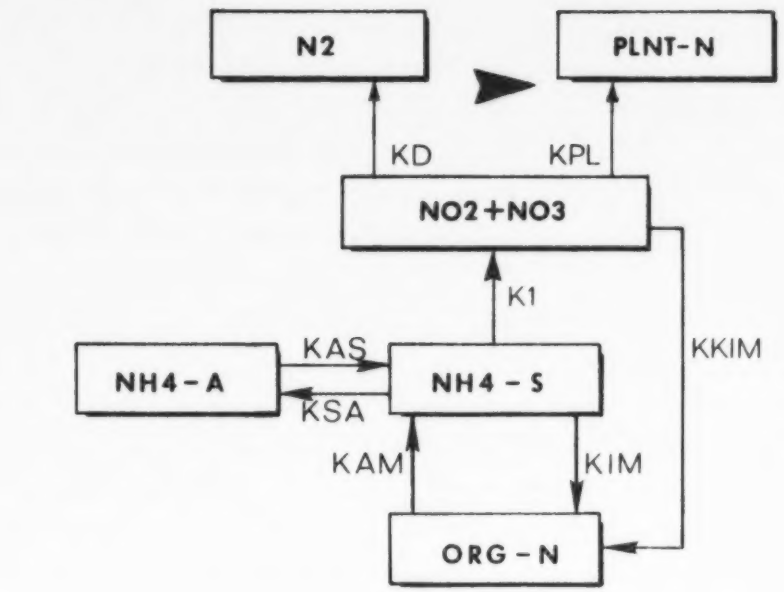
   These reactions take place in all four soil layers, and are simulated using first-order temperature corrected reaction rates. Any reaction path can effectively be eliminated by assigning a zero reaction rate to it.

2. As a consequence of the above, nutrient simulation involves advection of several substances. The dissolved materials, which must be advected over and through the soil, are:

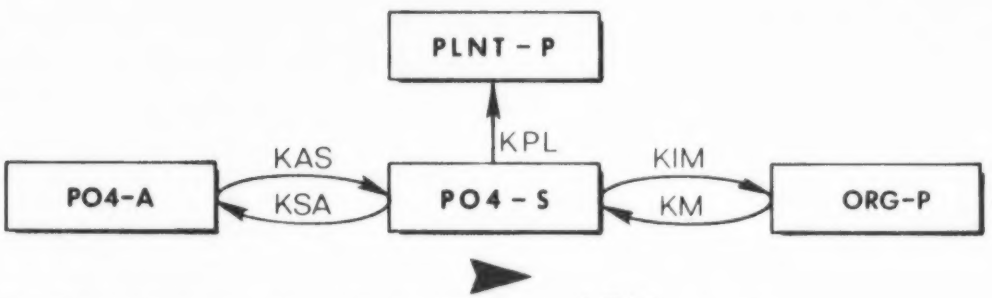
   NO2+NO3
   NH4-Solution
   PO4-Solution

In addition, washoff of the following particulate forms (associated with sediment) occurs from the surface layer:

   NH4-Adsorbed
   Organic N



A. Nitrogen transformations in ARM model



B. Phosphorus transformations in ARM model

FIGURE 25 Nutrient transformations in the ARM model

PO4-Adsorbed
Organic P

3. In both ARM and HSPF, the nutrient advection/reaction sequencing is different to that for pesticides. For nutrients, advection is performed every time step, starting at the surface and proceeding down to the groundwater layer. Reactions in each layer are calculated after advection is complete. In ARM there is a further complication; transformations due to reaction are performed intermittently. For example, the user can specify that this be done every 10 time steps. HSPF simulates reaction transformations every time step, but the user can specity how often the reaction rate should be recomputed.

   The difference in the way advection and reaction flux calculations are sequenced does have significant effect on the nutrient simulation results; this is discussed later.

Although the nitrogen, phosphorus and tracer sections of module PERLND can be simulated independently, the results will all be discussed together. Figures 26 through 33 are a representative sample of the results obtained from the nutrient test runs.

Figure 26 shows that the quantity of sediment-associated NH4 removal, simulated by the two models, agrees quite closely. The fact that this was also true for other forms of sediment-associated nutrients is confirmed by Figures 28, 29, 31, 32, and 33, which show the quantities removed in the storms of August 13, and 27, 1974. The reason for the good agreement is simple: both models gave very similar results for the simulation of sediment (accumulation, detachment and removal). Also, they agreed closely on the total amount of sediment-associated nutrients (organic and adsorbed) present in the surface layer. Since these are the only factors that govern the removal of sediment-associated nutrients, agreement between results from

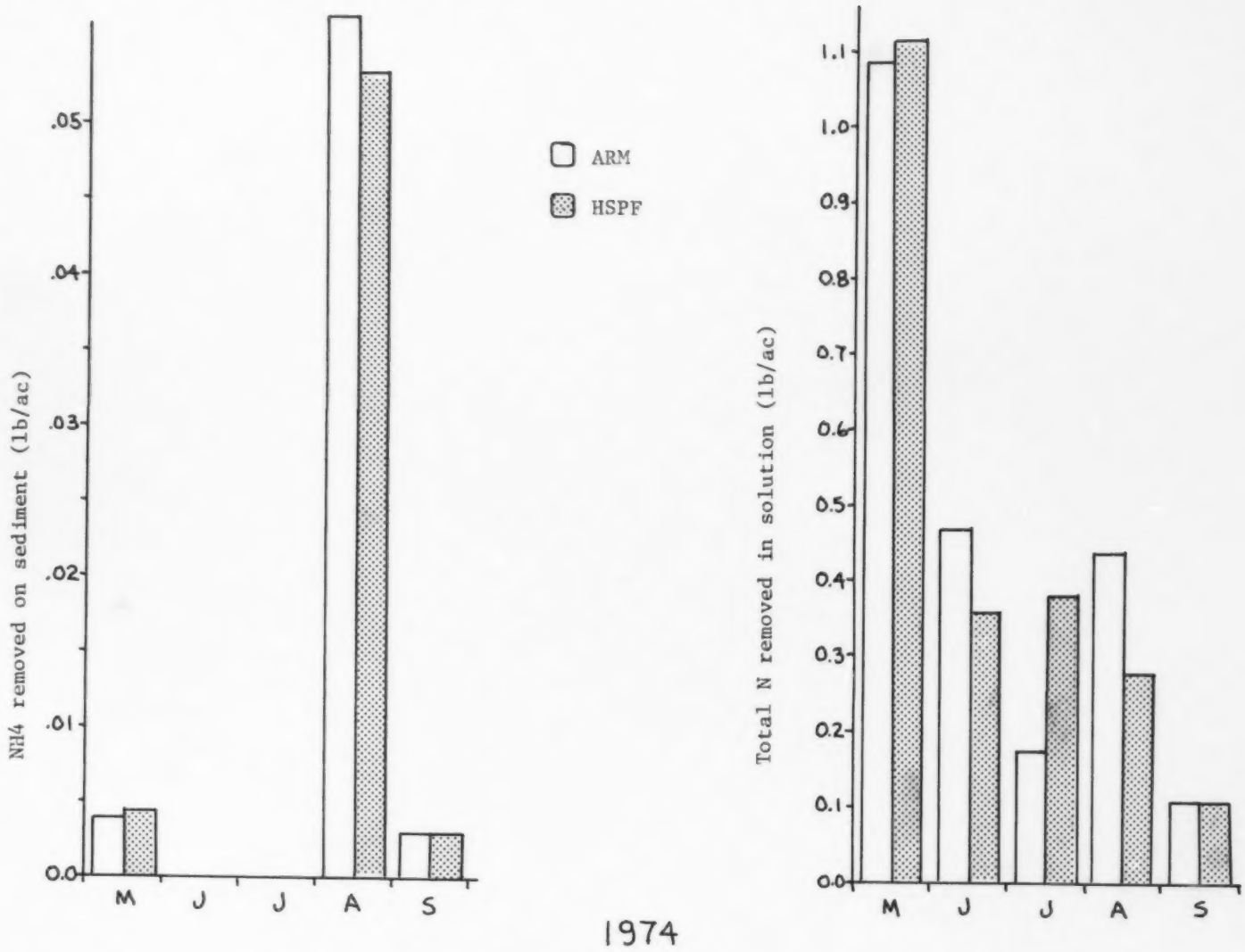


FIGURE 26 SIMULATED REMOVAL OF NITROGEN - P6 WATERSHED

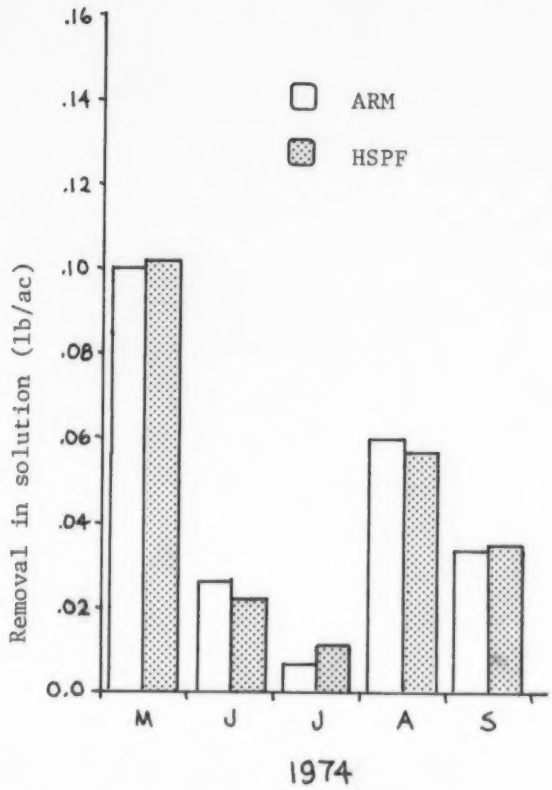


FIGURE 27 SIMULATED REMOVAL OF PHOSPHATE IN SOLUTION - P6 WATERSHED

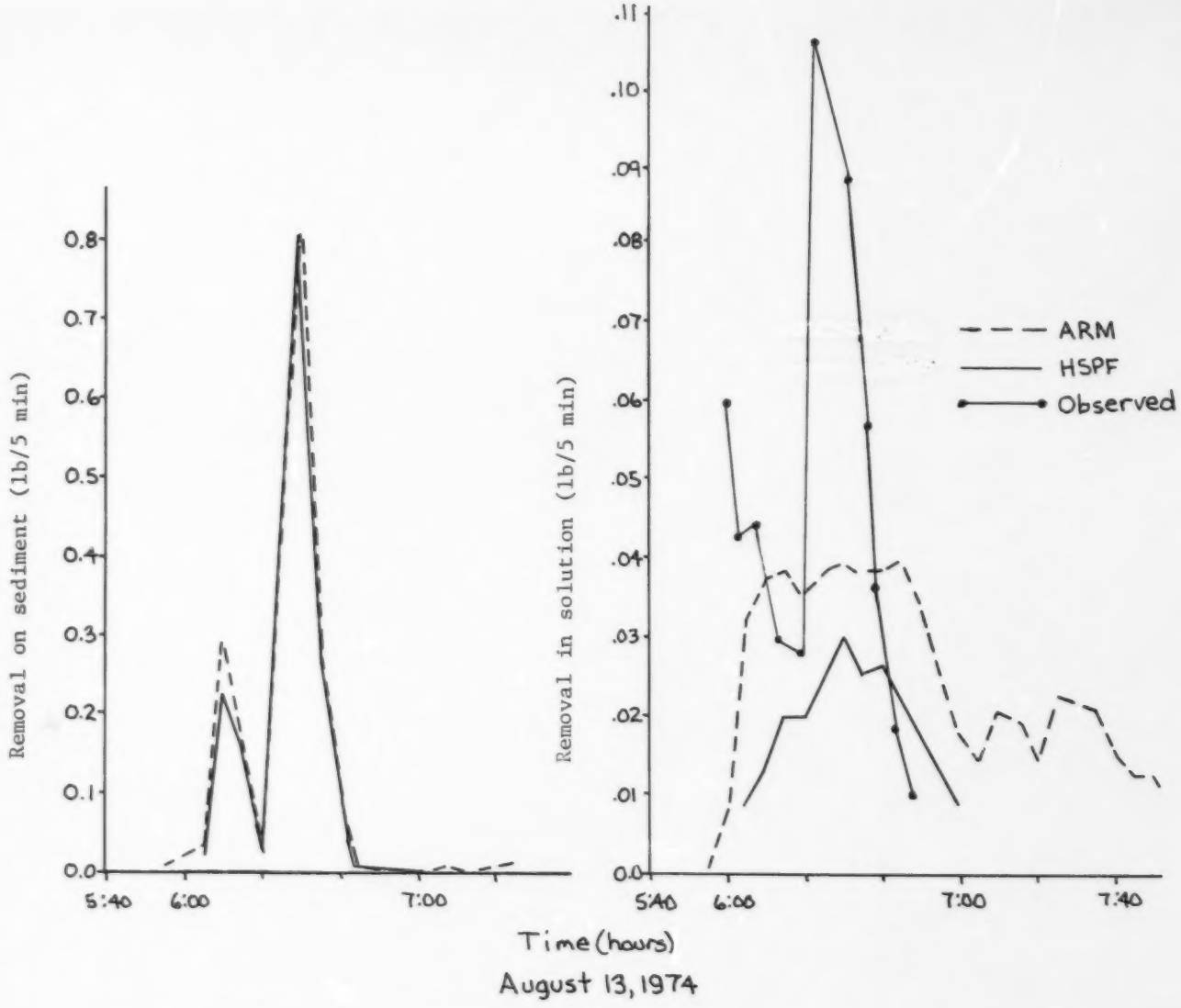


FIGURE 28 SIMULATED TOTAL REMOVAL OF NITROGEN FOR STORM OF AUGUST 13, 1974 - P6 WATERSHED

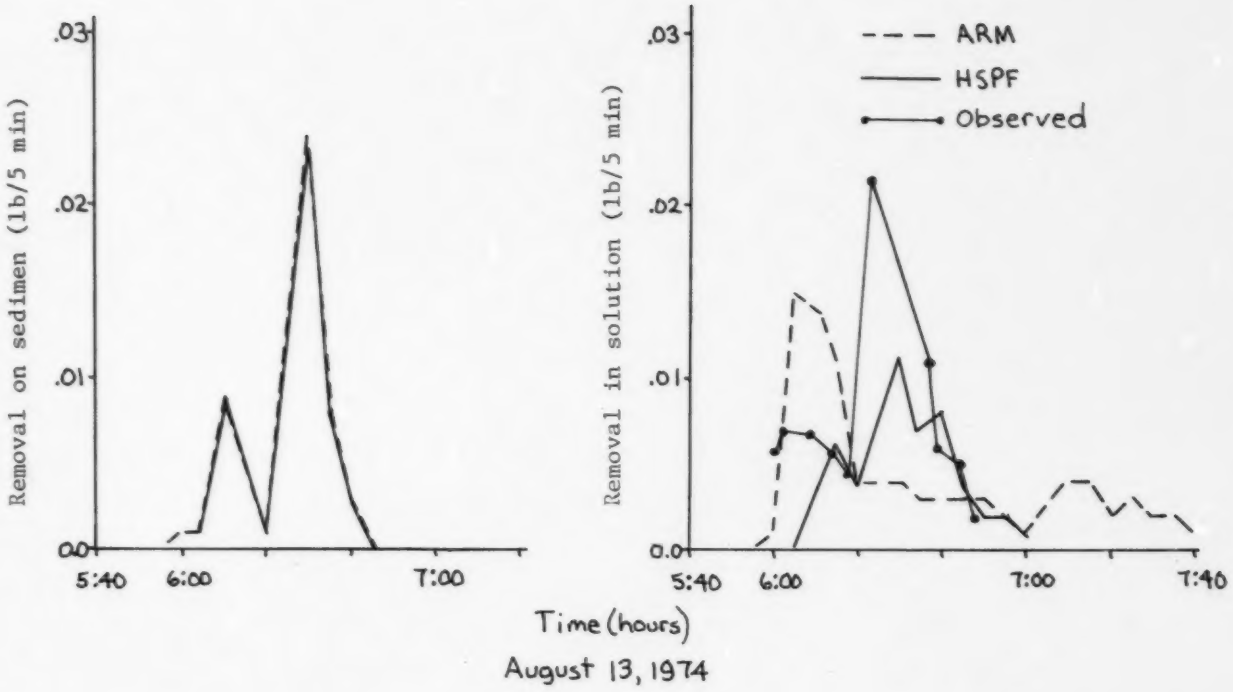


FIGURE 29 SIMULATED REMOVAL OF NH4, FOR STORM OF AUGUST 13, 1974 - P6 WATERSHED

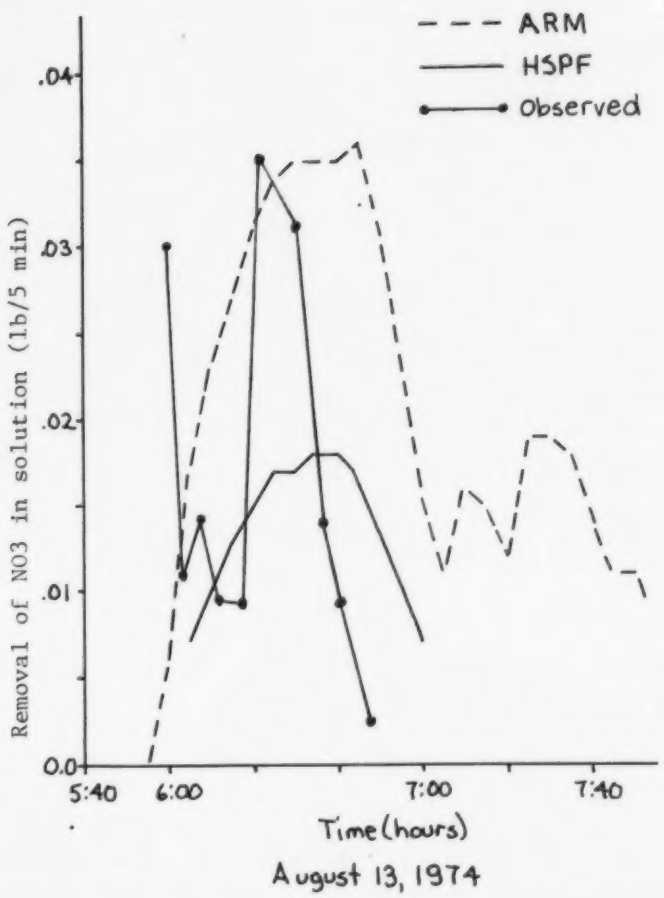


FIGURE 30 SIMULATED REMOVAL OF NITRATE, FOR STORM OF AUGUST 13, 1974 - P6 WATERSHED

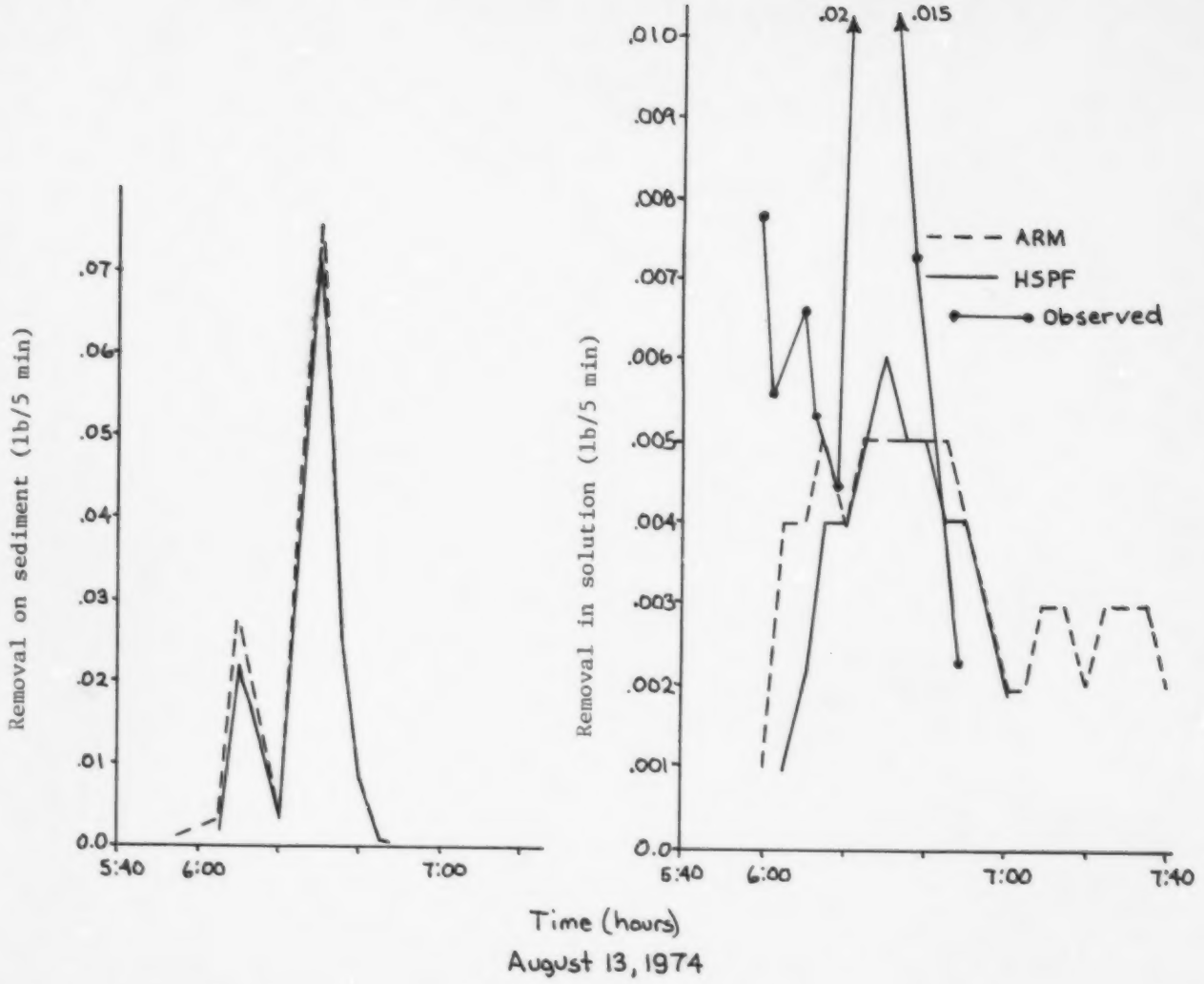


FIGURE 31 SIMULATED REMOVAL OF PHOSPHATE FOR STORM OF AUGUST 13, 1974 - P6 WATERSHED

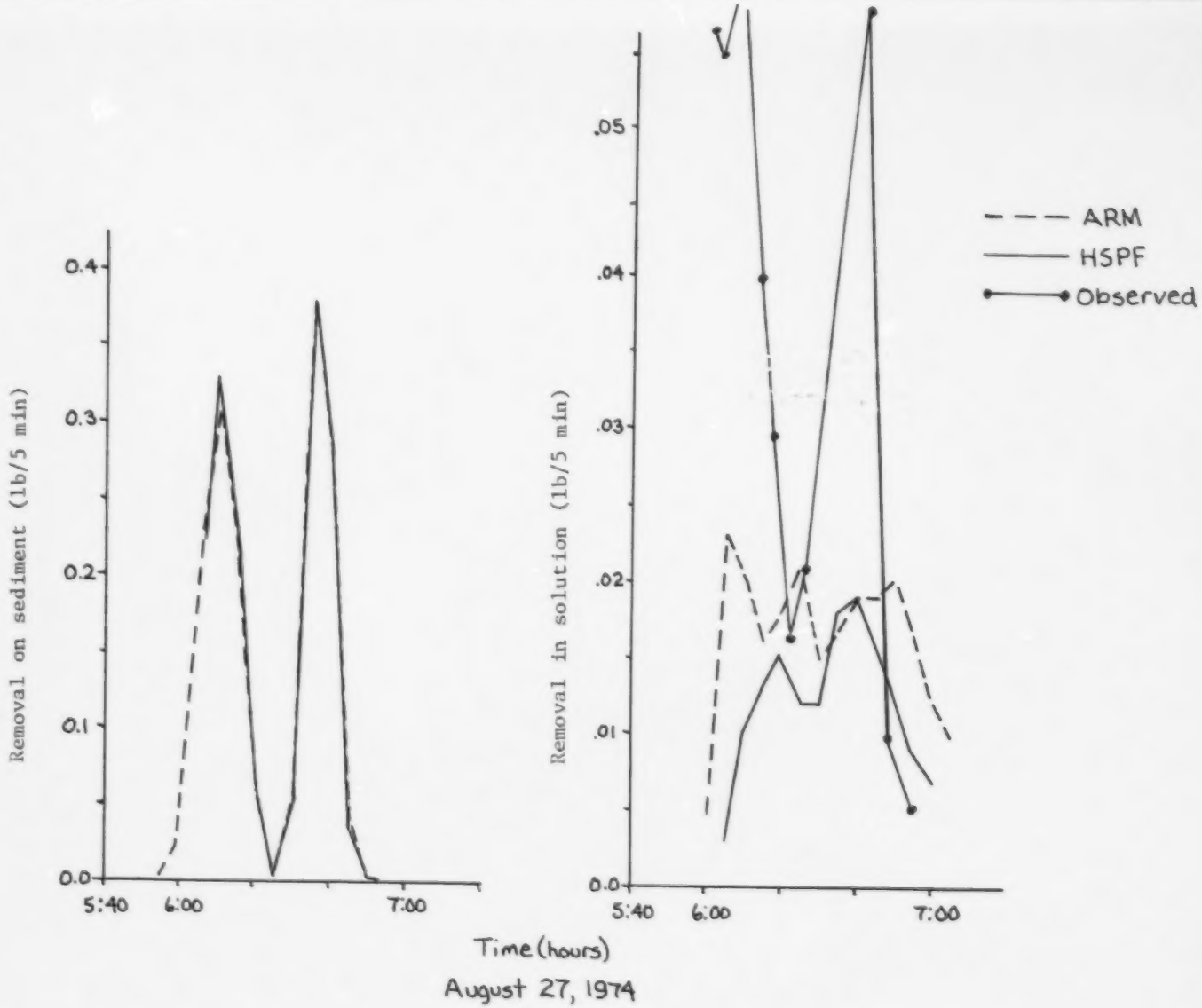


FIGURE 32 SIMULATED REMOVAL OF TOTAL N FOR STORM OF AUGUST 27, 1974 - P6 WATERSHED

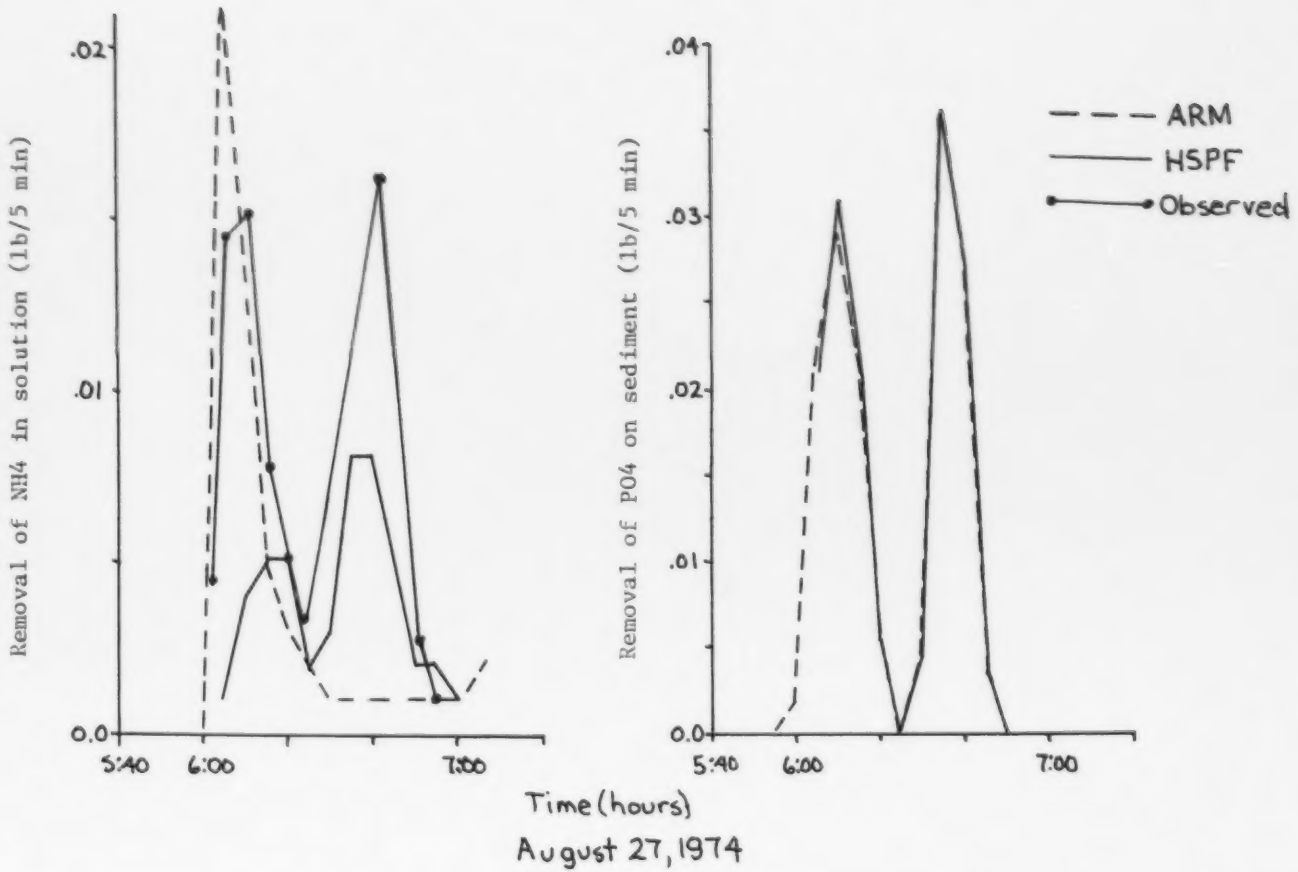


FIGURE 33 SIMULATED REMOVAL OF NH4 AND PO4 FOR STORM OF AUGUST 27, 1974 - P6 WATERSHED

the two models is assured.

In the case of dissolved constituents the story is, unfortunately, not as happy or as simple. Figures 26 through 33 show that there were often quite significant differences in output from the two models. Perhaps the most striking examples are the simulated removal of NH4 in solution, for the storms of August 13 and 27, 1974 (Figures 29 and 33).

In both cases ARM predicted initially high rates of removal, which rapidly tapered off. On the other hand, HSPF produced double-peaked curves. We attribute this difference to the fact that ARM performs reactions intermittently, in this case, every 12 time steps (i.e., once/hour). At the start of the storms (6 a.m. in both cases) there was an ample supply of NH4 in solution because an hour's worth of ammonification of organic N and desorption of adsorbed N had just been computed and the resulting fluxes added to the solution NH4 (Figure 25). Then, advection steadily removed the dissolved chemical during the storm and, because no replenishment due to reactions was computed until an hour later, the second peak flow rate (Figures 19 and 27) did not result in an associated peak in removal of dissolved NH4 (Figures 29 and 33). On the other hand, HSPF simulated both advection and reaction in each time step (although the reaction rates were altered only once per hour) so the exhaustion problem did not occur. Note that, for both storms, the general shape of the curve computed by HSPF is closer to that of the observed data than that produced by ARM. (By suitable adjustment of parameters, the HSPF outputs could be made to agree even better with the observations). Thus, we conclude that the continuous simulation of reaction fluxes (in HSPF) does result in a significant improvement over results obtained with ARM. Note that an ARM user can specify that reactions be computed more often, so this problem can be overcome.

We have already described how both models first advect material, between and out of the soil layers, and then simulate reactions within each layer (with the proviso that ARM usually handles reactions intermittently). Now, consider the behavior of the surface layer, which is usually regarded as very thin (in this case 0.125 in.). Because it is so thin, almost all the solutes present in it at the start of a time step will be advected down to the upper layer within that time step, in any significant storm. Usually, relatively small quantities are removed by surface runoff although, in HSPF, the ratio of percolation to surface runoff removal can be adjusted using the "surface layer percolation factor." If this adjustment is not made, most of the removal to the stream will be through the interflow path, which is the outlet from the upper layer. This can be seen in FIgures 28 through 31 in which the graphs showing removal of nutrients in solution, as simulated by HSPF for the storm of August 13, 1974, reflect the shape of the interflow, rather than the surface runoff, curve (Figure 34). However, the observed data, also plotted in these figures, are much closer to the shape of the surface runoff hydrograph than the interflow hydrograph (Figure 34). This problem affects both the ARM and HSPF models. It is recommended that one or both of the following measures be taken to overcome it:

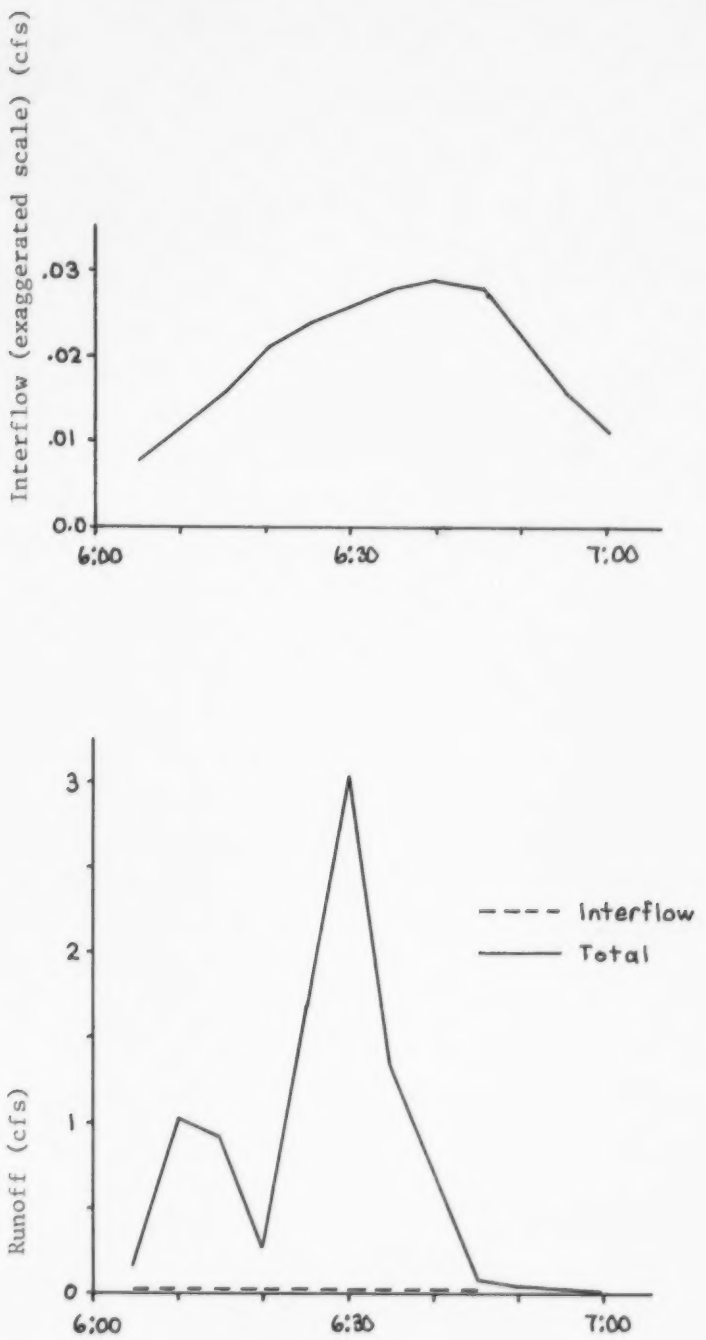


FIGURE 34 RUNOFF SIMULATED BY HSPF FOR STORM OF AUGUST 13, 1974 - P6 WATERSHED

1. Make the surface layer thicker, of the order of 1 to 4 inches. This should be coupled with a change to the code, to make the surface layer moisture storage a function not only of overland flow storage (as at present) but also of the upper zone storage. Indeed, it might be advisable to combine the present surface and upper layers into a single layer having two outflow paths--surface runoff and interflow. When this change is made, it should be coupled with some other changes to the MSTLAY Section of HSPF, designed to relax the present requirement that simulation of agricultural chemicals be limited to time steps of 5 or 15 minutes.

2. Use the surface layer percolation factor to promote more washoff of dissolved chemicals with surface runoff, rather than have them percolate vertically.

One further point. It was noticed that both the ARM and HSPF models simulated zero plant uptake of N and P from the surface layer. This is also a consequence of the thin surface layer. The only source of plant N (in ARM) is NO3 (Figure 25). And, the only way NO3 appears in the surface layer is:

1. by direct application
2. by oxidation of dissolved NH4

Since, during a storm, most of the dissolved NH4 and NO3 is flushed down to the upper layer in a single time step, the quantities which reside in the surface layer are typically quite small. This is especially true for NO3, because it is derived from oxidation of NH4 which is itself subject to heavy flushing. Only a small quantity of NH4 is usually available for oxidation and, when it is converted to NO3, it is again subject to heavy flushing in the next time step. The typical concentration of NO3 in the surface layer

is, thus, even less than that for dissolved NH4.

These factors account for the negligible plant uptake of NO3 and PO4 from the surface layer. The ARM and HSPF models cannot maintain significant quantities of NO3 and dissolved PO4 in the surface layer, and there cannot be plant uptake if there are no available nutrients.

Again, it seems that the cure to the problem lies in thickening the surface layer or in combining it with the upper layer.

Conclusion

From the tests conducted using data from the P6 watrshed, we concluded that the following sections of the HSPF PERLND module do correctly implement the algorithms, as described in the User's Manual:

SNOW
PWATER, with NBLKS=5 and DELT=5 minutes
SEDMNT
PSTEMP
MSTLAY
PEST
NITR
PHOS
TRACER

The testing program did, however, raise questions about the adequacy of the way the near-surface region of the soil is simulated, in both the HSPF and ARM models.

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